**PCT** WORLD INTELLECTUAL PROPERTY ORGANIZATION
International Bureau

INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(51) International Patent Classification 6 : C07K 1/00 — A2

(11) International Publication Number: **WO 98/38208**

(43) International Publication Date: 3 September 1998 (03.09.98)

(21) International Application Number: PCT/US98/03951

(22) International Filing Date: 27 February 1998 (27.02.98)

(30) Priority Data:
08/808,804 28 February 1997 (28.02.97) US

(71) Applicant: BEARSDEN BIO, INC. [US/US]; 34 Mt. Pleasant Drive, Aston, PA 19014 (US).

(72) Inventor: STURGESS, Michael; 42 Country Road, Perkasie, PA 18944 (US).

(74) Agent: PABST, Patrea, L.; Arnall Golden & Gregory, LLP, 2800 One Atlantic Center, 1201 W. Peachtree Street, Atlanta, GA 30309-3450 (US).

(81) Designated States: CA, JP, European patent (AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE).

**Published**
*Without international search report and to be republished upon receipt of that report.*

(54) Title: METHOD OF DETERMINING PROTEIN-LIGAND INTERACTIONS VIA COMPUTER MODELING

(57) Abstract

Disclosed is a method of determining receptor-ligand affinities by constructing a receptor protein model, placing a ligand into the binding pocket portion of the receptor protein model, calculating the protein-ligand interaction energies and then predicting the ligand binding affinity for the receptor protein from a mathematical equation. This method provides for a way of determining receptor binding affinities of potential ligand molecules without the need of actually preparing these molecules in a laboratory and testing them by *in vitro* receptor binding assays. Such determinations are useful for identifying potential ligands of receptors for use in studying receptor binding, in studying receptor activities, as potential modulators of receptor activity, and as actual or lead compunds useful as therapeutics which modulate receptor activity.

*FOR THE PURPOSES OF INFORMATION ONLY*

Codes used to identify States party to the PCT on the front pages of pamphlets publishing international applications under the PCT.

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **AL** | Albania | **ES** | Spain | **LS** | Lesotho | **SI** | Slovenia |
| **AM** | Armenia | **FI** | Finland | **LT** | Lithuania | **SK** | Slovakia |
| **AT** | Austria | **FR** | France | **LU** | Luxembourg | **SN** | Senegal |
| **AU** | Australia | **GA** | Gabon | **LV** | Latvia | **SZ** | Swaziland |
| **AZ** | Azerbaijan | **GB** | United Kingdom | **MC** | Monaco | **TD** | Chad |
| **BA** | Bosnia and Herzegovina | **GE** | Georgia | **MD** | Republic of Moldova | **TG** | Togo |
| **BB** | Barbados | **GH** | Ghana | **MG** | Madagascar | **TJ** | Tajikistan |
| **BE** | Belgium | **GN** | Guinea | **MK** | The former Yugoslav Republic of Macedonia | **TM** | Turkmenistan |
| **BF** | Burkina Faso | **GR** | Greece | | | **TR** | Turkey |
| **BG** | Bulgaria | **HU** | Hungary | **ML** | Mali | **TT** | Trinidad and Tobago |
| **BJ** | Benin | **IE** | Ireland | **MN** | Mongolia | **UA** | Ukraine |
| **BR** | Brazil | **IL** | Israel | **MR** | Mauritania | **UG** | Uganda |
| **BY** | Belarus | **IS** | Iceland | **MW** | Malawi | **US** | United States of America |
| **CA** | Canada | **IT** | Italy | **MX** | Mexico | **UZ** | Uzbekistan |
| **CF** | Central African Republic | **JP** | Japan | **NE** | Niger | **VN** | Viet Nam |
| **CG** | Congo | **KE** | Kenya | **NL** | Netherlands | **YU** | Yugoslavia |
| **CH** | Switzerland | **KG** | Kyrgyzstan | **NO** | Norway | **ZW** | Zimbabwe |
| **CI** | Côte d'Ivoire | **KP** | Democratic People's Republic of Korea | **NZ** | New Zealand | | |
| **CM** | Cameroon | | | **PL** | Poland | | |
| **CN** | China | **KR** | Republic of Korea | **PT** | Portugal | | |
| **CU** | Cuba | **KZ** | Kazakstan | **RO** | Romania | | |
| **CZ** | Czech Republic | **LC** | Saint Lucia | **RU** | Russian Federation | | |
| **DE** | Germany | **LI** | Liechtenstein | **SD** | Sudan | | |
| **DK** | Denmark | **LK** | Sri Lanka | **SE** | Sweden | | |
| **EE** | Estonia | **LR** | Liberia | **SG** | Singapore | | |

# METHOD OF DETERMINING PROTEIN-LIGAND INTERACTIONS VIA COMPUTER MODELING

## BACKGROUND OF THE INVENTION

The present invention generally relates to the field of protein topographical models and specifically to the use of receptor protein topographical models to determine the affinity of ligands for the modelled receptor protein.

Current knowledge of protein secondary structures and the factors governing the stability of such structures indicates that large complex proteins are composed of separate and essentially independent domains, which fold according to factors inherent in the amino acid sequence of the separate domains. Thus domains of proteins that are evolutionarily, but not functionally related, can fold into shapes that are topographically similar (Sonnhammer and Kahn, *Protein Sci.* 3:482-492 (1994)).

The folding patterns of the protein backbone of bacterial periplasmic binding proteins reveal a surprising similarity in the topography of the protein structures. They all exhibit a bilobic architecture. Generally the topography of the individual lobes follows the same design wherein the protein sequence forms alternatively $\beta$-strand and $\alpha$-helical arrays which are arranged in opposing directions. Each lobe is formed by a central parallel stranded $\beta$-sheet at its core and a series of $\alpha$-helical sequences surrounding the central core. The ligand binding site within these proteins is formed by the upper surface of lobe I and the lower surface of lobe II. This architecture can be seen in leucine/alanine/ornithine-binding protein (LAOBP; Oh *et al.*, *J. Biol. Chem.* 268:11384-11355 (1993)), arabinose-binding protein (ABP; Quiocho and Vyas, *Nature* 310:381 (1984)), galactose-binding protein (GBP; Vyas *et al.*, *Science* 242:1290-1295 (1988); Mowbray *et al.*, *Receptor* 1:41-54 (1990)), maltose-binding protein (MBP; Spurlino *et al.*, *J. Biol. Chem.* 266:5202-5219 (1991)), and sulfate-binding protein (SBP; Pflugrath and Quiocho, *J. Mol. Biol.* 200:163-180 (1988)). The location

of the ligand binding site places the ligand in contact with the loop regions of the proteins which connect the highly conserved β-strands and α-helices. Analogous loop regions are seen to interact with the bound ligand in all the structures of these bacterial periplasmic binding proteins.

Two theories may be proposed to rationalize such topographical similarities inherent in this family of proteins. If all such bacterial periplasmic binding proteins were evolutionarily derived from common ancestral proteins it would be expected that the functional binding pockets were conserved throughout the process of evolution. Consequently it should not be surprising that the ligand binding site for ligands as diverse as sugars, amino acids and polyanionic oxyanions would share the same topographical features and only differ in the protein side chains presented to the ligands. Alternatively, it may be argued that these proteins are not derived from a common ancestor, but instead have evolved to a common topography which is unusually efficient in the binding of individual ligands.

Irrespective of the evolutionary driving force, the topographical features which form the ligand binding pocket in periplasmic binding proteins are very highly conserved. Furthermore, these same features can be identified in a range of ligand binding sites from other families of proteins. The mononucleotide binding pocket, which is common to a large family of kinases and phosphatases, has been often recognized in an uncharacterized protein by the presence of two amino acid sequences known as the Walker A and B motifs (Walker *et al.*, *EMBO J.* 1:945-951 (1982); Hasemann *et al.*, *Structure* 4:1017-1029 (1996)). These motifs are highly conserved amino acid sequences which are directly involved in the binding of the mononucleotide ligand. The location of these motifs within such proteins is consistent with the topography of the bacterial periplasmic binding protein ligand binding site, suggestive of a topographical similarity within these families of proteins.

Additionally, recent work by Quiocho has shown that the family of DNA repressor proteins exemplified in the *Lac* repressor and the *Gal*

repressor have essentially topographically identical repressor ligand binding sites to the sugar binding variants of the bacterial periplasmic binding proteins. This comparison has recently been verified by crystallographic analysis of these proteins both with and without bound repressor ligands. Indeed, not only are the binding sites in these proteins highly comparable, but the mechanism of action of the individual proteins is essentially the same (ligand binding may either induce or inhibit a closing of the bilobic structure in a manner that has been compared to a "Venus Fly-trap"; Quiocho, *Phil. Trans. R. Soc. Lond.* B 326:341-351 (1990)).

It has been suggested that the ligand binding domain of the metabotropic glutamate receptors (mGluR1-9), a family of G-protein coupled membrane bound receptors, is comparable to the topography of the bacterial periplasmic binding protein leucine/isoleucine/valine binding protein (LIVBP); O'Hara *et al.*, *Neuron* 11:41-52 (1993). A detailed model of the ligand binding domain of mGluR1 has recently been proposed in O'Hara *et al.* based upon the known structural coordinates of LIVBP. These correlations are strong evidence for evolutionary derivation of these families of proteins from a common parent, (Figure 1).

Employing a similar comparative approach to that outlined above, Nakanishi (Nakanishi *et al.*, *Neuron* 5:569 (1990)) was the first to suggest that the ionotropic glutamate receptor proteins, even though much larger and more complex, may share the same topography of the ligand binding site as the bacterial periplasmic binding proteins. He suggested that the ionotropic glutamate receptor proteins are part of a much larger family of ligand-gated ion channel proteins comprising the nicotinic acetylcholine, $\gamma$-aminobutyric acid, glycine, and serotonin receptor proteins. Additional invertebrate derived ligand-gated ion channels, such as the invertebrate glutamate receptors, probably share a common topography with the vertebrate analogs.

Extensive analysis of the crystal structures of the bacterial periplasmic binding proteins allowed through comparison of these

structures to be made by Quiocho (Quiocho, *Curr. Opin. Struct. Biol.* 1:922 (1992); *Phil. Trans R. Soc. Lond. B* 326:341-351 (1990)). Although the sequence identity of this family of proteins is not necessarily high (often less than 30%) and the endogenous ligands are highly varied (sugars, cationic amino acids, neutral amino acids and polyanionic oxyanions such as sulfate), the proteins exhibit a common topographic frame work around which the binding domain structure is built. The ligand binding site in all members of this family of proteins is formed from the analogous "loop" regions of the protein between common $\beta$-strands and $\alpha$-helices. Remarkably, the preferred ligand varies considerably but the location of the binding site does not.

Excitatory neuronal transmission within the central nervous system (CNS) is mediated predominantly by ion flux through a family of cation selective ion channel complexes gated by the neurotransmitter L-glutamate. Subclassification of these protein complexes, based upon the pharmacological properties of a series of natural and unnatural agonists (Figure 2), has shown the family to be divided into two major subtypes: the N-methyl-(D)-aspartate (NMDA) receptors (NR1 and NR2) and the non-NMDA receptors. The latter group may be further divided into those specifically activated by 2(S)-amino-3-(5'-methyl-3'-hydroxyisoxazoline)-propionic acid (AMPA) (AMPA receptors, GluR1-4) and those preferentially activated by kainic acid (KA receptors, GluR5-7, KA1 and KA2; Sommer and Seeburg, *Trends in Pharmacol. Sci.* 13:291-296 (1992)).

Compounds which inhibit NMDA and AMPA receptors have been shown to be effective neuroprotectants under conditions of ischemic insult and additionally have potential in the treatment of conditions such as stoke, head trauma and epilepsy. Compounds which modulate the kainate receptor may be useful for the treatment of neuropathic pain. Efforts to find NMDA receptor antagonists and blockers which are neuroprotective in animal models have been very successful while efforts to find AMPA or KA antagonists, have been much less successful. A number of

pharmaceutical companies have pursued clinical development of ion channel blockers or full antagonists of the NMDA, AMPA and kainate receptors to protect against both chronic and acute neurodegenerative processes. Although, several compounds have entered clinical trails there has been only limited progress in developing a clinically useful NMDA or AMPA receptor antagonist because the compounds exhibit severe side effects ranging from hallucinations and loss of coordination, to neuronal damage, memory impairment, learning disability and nephrotoxicity. There still exists a need to find new compounds which can safely inhibit the function of NMDA, AMPA, or KA receptors. Key to the search for new compounds is determining which structures bind to which receptor and their binding affinity for that receptor.

Recently Nakanishi (Nakanishi *et al.*, *Neuron* 5:569 (1990)) suggested that the general topography of the agonist ligand binding site of ionotropic glutamate receptors is homologous to that of the bacterial periplasmic binding proteins. Many examples of these proteins have been analyzed by X-ray crystallography both with and without associated ligands. Actual comparison of the amino acid sequences of ionotropic glutamate receptors and the lysine/arginine/ornithine binding protein (LAOBP) shows a very low level of both sequence similarity (less than 30%) and identity (less than 15%) within the identified regions. Following Nakanishi's work, Stern-Bach *et al.* (Stern-Bach *et al.*, *Neuron* 13:1345 (1994)) concluded from a series of experiments involving GluR3/GluR6 chimeric proteins that the ligand binding domains of these proteins are topographically similar to the periplasmic binding protein LAOBP. A detailed study of chimeric GluR3/GluR6 receptors revealed a pattern of amino acid sequences which was shown to drive the AMPA/KA selectivity of these proteins. This pattern of sequences could be overlaid onto the known binding site of LAOBP, leading the authors to speculate that the agonist binding domain of the glutamate receptors and LAOBP display homologous tertiary structures. Construction of a simple homology model of this portion of the AMPA receptor, based upon the crystal structure of

LAOBP, generated a bilobic cartoon-like model of the agonist binding domain. The significance of this effort is diminished by key inaccuracies in the glutamate receptor sequences employed in the comparison with LAOBP. Sutcliffe (Sutcliffe *et al.*, *Biophysical J.* 70:1575 (1996)) has recently proposed a different alignment of the related KA receptors with LAOBP, and has constructed the analogous homology model. Sutcliffe suggested a highly novel glutamate binding mode for the NMDA receptor but did not show any details of the binding mode for glutamate and further did not suggest a predictive model for glutamate binding.

It is therefore an object of the present invention to provide a method of building a predictive binding protein model based on topographical similarity to a binding protein of known structure.

It is also and object of the present invention to provide a method of predicting the affinity of a potential ligand molecule for a binding protein.

It is also an object of the present invention to provide a method of predicting the selectivity of a potential ligand molecule for a family of related binding proteins in order to reduce unwanted side effects.

## BRIEF SUMMARY OF THE INVENTION

Disclosed is a method of determining receptor-ligand affinities by constructing a receptor protein model, placing a ligand into the binding pocket portion of the receptor protein model, calculating the protein-ligand interaction energies and then predicting the ligand binding affinity for the receptor protein from a mathematical equation. This method provides a way of determining receptor binding affinities of novel molecules without the need of actually preparing these molecules in a laboratory and testing them by *in vitro* receptor binding assays. Such determinations are useful for identifying novel receptor ligands, and actual or lead compounds useful as therapeutics which modulate receptor activity.

Specific examples of the disclosed method are provided. In one embodiment, a method is provided that allows the prediction of ligand

binding affinities to receptor proteins that contain bacterial amino acid periplasmic protein topographical binding domains. In another embodiment, a method is provided that allows the prediction of ligand binding affinities to receptor proteins that contain LAOBP topographical binding domains. In another embodiment, a method is provided that allows the prediction of NMDA, AMPA and KA receptor ligand binding affinities. The disclosed method allows such predictions by describing a protein topographical model of the ligand binding pocket of each receptor, building a predictive equation of binding affinity based upon a known basis set of molecules, placing a novel ligand in the pocket, calculating the energies of the bound and unbound protein and ligand, and fitting the results to a predictive equation.

In a preferred mode, the disclosed method is a computer based method for predicting the binding affinity of actual or potential ligand molecules to receptor proteins. Preferably, this can be accomplished by:

(1) building a model of a protein-ligand binding domain (also referred herein to as a ligand binding pocket) based upon the similarity of the receptor protein structural topography to bacterial amino acid periplasmic binding proteins,

(2) refinement of the protein-ligand binding domain model by energy minimization of the protein with a high affinity ligand in the binding pocket (the resulting protein-ligand binding domain model is also referred to herein as the receptor protein model),

(3) calculating a series of interaction energies ($E_{interact}$) by calculating the energies of the receptor protein model ($E_{receptor}$) and basis set molecules ($E_{molecule}$) individually, and the total energies of the individual bound complexes formed from the protein and basis set molecules ($E_{receptor+molecule}$), as shown in equation 1,

$$E_{interact} = E_{receptor+molecule} - (E_{receptor} + E_{molecule}) \quad \text{(Eq. 1)}$$

(4) generating a predictive equation, such as equation 2, by doing a regression analysis on the basis set,

$$\text{Ligand Affinity} = -xE_{interact} + y\text{Mol.Charc.}_{ligand} - z\text{Mol.Charc.}_{ligand} + N \quad \text{(Eq. 2)}$$

where $\text{Mol.Charc.}_{ligand}$ is a molecular characteristic and x, y, z, and N are the regression parameters,

(5) calculating the interaction energy ($E_{interact}$*) for a potential ligand molecule by calculating energies of the receptor protein model ($E_{receptor}$) and potential ligand molecule ($E_{molecule}$*) individually and the energy of the individual bound complex formed from the protein and the potential ligand molecule ($E_{receptor+molecule}$*), as shown in equation 3, and

$$E_{interact}^* = E_{receptor+molecule}^* - (E_{receptor} + E_{molecule}^*) \quad \text{(Eq. 3)}$$

(6) fitting the data for the difference in the energies ($E_{interact}$*) and other molecular characteristics such as, molecular volume and number of rotatable bonds to the predictive equation, equation 2.

It is specifically contemplated that where a model of a protein-ligand binding domain already exists, or where such a model has been built in a different manner or from different information than in the first step above, the method can be practiced by performing remaining steps (for example, steps 2 through 6 above) using such a model. It is also specifically contemplated that once a predictive equation has been generated for a given protein-ligand binding domain model (using, for example, steps 1 through 4, or 2 through 4, above), the method can be practiced by performing the remaining steps (for example, steps 5 and 6 above) using the predictive equation and the model. It is also specifically contemplated that the various steps of any of the modes in the disclosed method need not be performed in any specific time frame to constitute practice of the disclosed method. Thus, for example, the various steps can be performed at different times and in different locations while still collectively constituting practice of the method.

Without being limited to any particular theory, the disclosed method is based in part on the realization that, while the overall

topography of complete ligand-gated ion channel proteins is known to vary with the number of transmembrane regions inherent in these proteins (leading to the C-terminal domain of these proteins being either intra- or extracellular), sequence similarities in the regions shown to influence ligand binding suggest a common topography for the ligand binding domains of these proteins. Thus, it was realized that all ionotropic glutamate receptors, such as those discussed in Examples 1 through 4, are likely members of a much larger class of ligand-gated ion channel associated receptor proteins.

## BRIEF DESCRIPTION OF THE DRAWINGS

Figure 1 is a diagram showing the possible evolutionary relationship of the bacterial periplasmic binding protein related proteins to sugar and oxyanion binding proteins. In this diagram, AMPA refers to 2(S)-amino-3-(5'-methyl-3'-hydroxyisoxazoline)-propionic acid, GABA refers to $\gamma$-aminobutyric acid, nACh refers to nicotinic acetylcholine, 5-$HT_3$ refers to class 3 5-hydroxytrptamine (serotonin) receptor, LAOBP refers to lysine/ arginine/ornithine binding protein, LIVBP refers to the bacterial periplasmic binding protein LIVBP, mGluRs refers to metabotropic glutamate receptors, GalBP refers to galactose binding protein, and MalBP refers to maltose binding protein.

Figure 2 is a diagram showing the structures of ligands which activate ionotropic excitatory amino acid receptors. Specifically, the structures of L-glutamate, N-methyl-(D)-aspartate (NMDA), 2(S)-amino-3-(5'-methyl-3'-hydroxyisoxazoline)-propionic acid (S-AMPA), and kainic acid are depicted.

Figure 3 is a diagram showing the structures of fifteen molecules which make up the GluR3 model basis set of molecules, and a sixteenth molecule used to test the GluR3 model and predictive equation.

Figure 4 is a diagram showing the structures of molecules which make up the of KA receptor model basis set of molecules and a molecule used as a potential ligand molecule. These are designated, in order, L-

Glu, SYM 2081, SYM 2048, SYM 2077, SYM 2047, SYM 2084, SYM 2072, SYM 2194, SYM 2139 and SYM 2114. The potential ligand molecule is designated SYM 2083.

Figures 5A, 5B, 5C, and 5D are a table showing the alignment of amino acids in LAOBP (SEQ ID NO:1), NR1-Z (SEQ ID NOs:2 and 3), NR2-C (SEQ ID NOs:4 and 5), NR2-B (SEQ ID NOs:6 and 7), NR2-A (SEQ ID NOs:8 and 9), GluR3 (amino acids 4 to 123 of SEQ ID NO:10 and amino acids 2 to 150 of SEQ ID NO:11), and GluR6 (amino acids 4 to 123 of SEQ ID NO:12 and amino acids 2 to 146 of SEQ ID NO:13). Consensus segments are also shown (SEQ ID NOs:14 through 25).

Figures 6A and 6B are a table showing the alignment of amino acids in LAOBP (SEQ ID NO:1), GluR3 (amino acids 1 to 120 of SEQ ID NO:10 and amino acids 1 to 149 of SEQ ID NO:11), and GluR6 (amino acids 1 to 120 of SEQ ID NO:12 and amino acids 1 to 145 of SEQ ID NO:13).

## DETAILED DESCRIPTION OF THE INVENTION

### A. Definitions

The disclosed method can be understood by reference to the following definitions.

Basis Set: A set of three or more molecules that binds to the receptor protein of interest for which experimentally determined binding affinities spanning a range of at least 2 log units are known.

Potential Ligand Molecule: A molecule of interest for which the binding characteristics to a binding protein are to be calculated using the disclosed method.

Topographical: Relating to the spatial relationship of physical features of a place or region of a protein.

Topographical similarity: Similarity of the spatial relationships of physical features of a place or region of one protein with those of another protein.

Ionotropic Receptors: A protein which either individually or by oligomerization with other proteins forms an ion channel.

AMPA: 2(S)-amino-3-(5'-methyl-3'-hydroxyisoxazoline)-propionic acid.

AMPA receptor: A postsynaptic or pre-synaptic receptor which is stimulated, at a minimum, by the excitatory amino acid glutamic acid as well as by AMPA. It is a ligand-gated ionotropic receptor.

Stimulation of a receptor: Activation of a receptor protein so as to induce a functional change in the protein resulting in a change in a measurable physiological property of the protein associated with the native function of that protein.

Kainate Receptor: A postsynaptic or presynaptic receptor which is stimulated, at a minimum, by the excitatory amino acids glutamic acid as well as by kainic acid, but is not stimulated by NMDA or AMPA. It is a ligand-gated ionotropic receptor.

Ligand Affinity: A measure of how tightly a molecule binds to a protein relative to another molecule. Higher (or greater) affinity indicates tighter binding.

NMDA: N-methyl-(D)-aspartate.

NMDA Receptor: A postsynaptic or pre-synaptic receptor which is stimulated, at a minimum, by the excitatory amino acid glutamic acid as well as by NMDA, but is not stimulated by AMPA or kainic acid. It is a ligand-gated ionotropic receptor.

NMDA receptor glutamate site: A ligand binding site present on NMDA receptor proteins which binds L-glutamic acid and NMDA.

NMDA receptor glycine site: A ligand binding site present on NMDA receptor proteins which binds glycine and not glutamate or NMDA.

$E_{receptor}$: The energy of a receptor protein model calculated from an ensemble of atoms representing the receptor protein model using a Force Field such as CHARMM (Brooks *et al.*, *J. Comp. Chem.* 4:187-217

(1983), MM1, or MM2 (Kao and Allinger, *J. Am. Chem. Soc.* 99:975 (1972)).

Force field: A series of parameters representative of the various attractive and repulsive components of the interaction between two atoms (See, for example, Kao and Allinger).

$E_{molecule}$: The energy of a molecule calculated from an ensemble of atoms representing the molecule using a Force Field such as CHARMM, MM1, or MM2.

$E_{receptor+molecule}$: The total energy of a bound complex formed from a protein and molecule calculated from an ensemble of atoms representing the bound complex using a Force Field such as CHARMM, MM1, MM2.

$E_{molecule}$*: The energy of a potential ligand molecule calculated from an ensemble of atoms representing the potential ligand molecule using a Force Field such as CHARMM, MM1, or MM2.

$E_{receptor+molecule}$*: The total energy of a bound complex formed from a protein and potential ligand molecule calculated from an ensemble of atoms representing the bound complex using a Force Field such as CHARMM, MM1, MM2.

Mol. Charc.: A molecular characteristic such as, but not limited to, molecular volume, number of rotatable bonds, molar refractivity, and dipole moment.

Computer based: In reference to a method, a method in which at least some of the steps are carried out with, or facilitated by a computer. In reference to a model, a model in which a representation of the structure of the modelled object is contained in a computer. Such a model is also referred to herein as a computer model.

**B. Method**

A general form of the disclosed method involves a series of specific steps which result in the generation of a model of a protein-ligand binding domain, generation of a predictive equation for the energy of protein-ligand complexes, and fitting the calculated energy of a complex of the protein and a potential ligand molecule to the predictive equation.

In a preferred mode, the disclosed method is a computer based method for predicting the binding affinity of actual or potential ligand molecules to receptor proteins. Preferably, this can be accomplished by:

(1) building a model of a protein-ligand binding domain (also referred herein to as a ligand binding pocket) based upon the similarity of the receptor protein structural topography to bacterial amino acid periplasmic binding proteins,

(2) refinement of the protein-ligand binding domain model by energy minimization of the protein with a high affinity ligand in the binding pocket (the resulting protein-ligand binding domain model is also referred to herein as the receptor protein model),

(3) calculating a series of interaction energies ($E_{interact}$) by calculating the energies of the receptor protein model ($E_{receptor}$) and basis set molecules ($E_{molecule}$) individually, and the total energies of the individual bound complexes formed from the protein and basis set molecules ($E_{receptor+molecule}$), as shown in equation 1,

$$E_{interact} = E_{receptor+molecule} - (E_{receptor} + E_{molecule}) \quad \text{(Eq. 1)}$$

(4) generating a predictive equation, such as equation 2, by doing a regression analysis on the basis set,

$$\text{Ligand Affinity} = -xE_{interact} + y\text{Mol.Charc.}_{ligand} - z\text{Mol.Charc.}_{ligand} + N \quad \text{(Eq. 2)}$$

where $\text{Mol.Charc.}_{ligand}$ is a molecular characteristic and x, y, z, and N are the regression parameters,

(5) calculating the interaction energy ($E_{interact}$*) for a potential ligand molecule by calculating energies of the receptor protein model ($E_{receptor}$) and potential ligand molecule ($E_{molecule}$*) individually, and the energy of the individual bound complex formed from the protein and the potential ligand molecule ($E_{receptor+molecule}$*), as shown in equation 3, and

$$E_{interact}^* = E_{receptor+molecule}^* - (E_{receptor} + E_{molecule}^*) \quad \text{(Eq. 3)}$$

(6) calculating the affinity of the potential ligand molecule by fitting the data for the difference in the energies ($E_{interact}$*) and other

molecular characteristics such as molecular volume and number of rotatable bonds to the predictive equation, equation 2.

The method can also be practiced using an existing model, or a model built in a different manner or from different information than in the first step above. The method can also be practiced using a predictive equation which has been previously generated for a given protein-ligand binding domain model. That is, practice of the disclosed method does not require that a model be built or a predictive equation generated each time the binding characteristics of a potential ligand are to be determined using the method. In fact, it is preferred that a model be built and a predictive equation generated only once, while the model, the predictive equation, or both, are used numerous times for numerous potential ligand molecules. Such multiple and subsequent use of the results of the early steps of the disclosed method is considered to be an extension or continuation of the earlier steps and, in ultimate combination with the earlier steps, to constitute an individual instance of the full method.

**1. Building A Model.**

It is preferred that an initial model of a protein-ligand binding domain of a receptor of interest be built by reference to a related bacterial amino acid periplasmic binding protein. This is preferably accomplished by first aligning the receptor to a bacterial amino acid periplasmic binding protein. An example of such an alignment, specifically alignment of glutamate receptor ligand binding sites with LAOBP, is discussed by Stern-Bach *et al.* (*Neuron* 13:1345 (1994)) and is shown in Figure 5. The alignment can be adjusted if there is a high variance in regression analysis used for generating the predictive equation.

An alignment such as is shown in Figure 5 indicates the possible presence of an evolutionarily conserved ligand binding domain. A topographical model of a protein can then be constructed based upon the crystal structure of the bacterial amino acid periplasmic binding protein and the above alignment. Preferred bacterial binding proteins are leucine/alanine/ornithine-binding protein (LAOBP; Oh *et al.*, *J. Biol.*

*Chem.* 268:11384-11355 (1993)), arabinose-binding protein (ABP; Quiocho and Vyas, *Nature* 310:381 (1984)), galactose-binding protein (GBP; Vyas *et al.*, *Science* 242:1290-1295 (1988); Mowbray *et al.*, *Receptor* 1:41-54 (1990)), maltose-binding protein (MBP; Spurlino *et al.*, *J. Biol. Chem.* 266:5202-5219 (1991)), and sulfate-binding protein (SBP; Pflugrath and Quiocho, *J. Mol. Biol.* 200:163-180 (1988)), ribose receptor-binding protein (RBP; Mowbray and Cole, *J. Mol. Biol.* 225:155-175 (1992)), leucine/isoleucine/valine-binding protein (LIVBP; Sack *et al.*, *J. Mol. Biol.* 206:171-191 (1989), leucine-binding protein (LBP; Sack *et al.*, *J. Mol. Biol.* 206:193-207 (1989), and PotD (Sugiyama *et al.*, *J. Biol. Chem.* 271:9519 (1996). The model can be constructed using any suitable medium or structural convention. It is preferred that the model be constructed employing a commercially available computer protein modeling package such as "Quanta v4.0" (Molecular Simulations Incorporated), or "Discover" (Tripos Incorporation). Such modeling programs and their general use are known to those of skill in the art. It is specifically contemplated that any computer based protein modeling system which can be used to calculate molecular energies is suitable for use in, and is a preferred medium for practicing, the disclosed method. Those regions of the protein hypothesized to adopt a secondary structure topographically similar to the bacterial amino acid periplasmic binding protein are modelled by duplicating those regions of the template protein. In the disclosed method, it is preferred that this is done primarily through alignment of the protein to a bacterial periplasmic binding protein (although any additional information regarding either the structure of the protein or the similarity of the structure to the bacterial protein can also be used). Conversely, those sequences of the protein that are additional to, or different from, the basic template structure (of the bacterial protein) can be analyzed according to the standard algorithms for predicting protein secondary structure (Holley and Karplus, *Proc. Natl. Acad. Sci. USA* 86:152-156; LaRosa *et al.*, *Science* 249:932-935 (1990); Garnier *et al.*, *J. Mol. Biol.* 120:97-120 (1978)). With such tendencies in mind, these

sequences can be modeled by comparison to a protein structural library, such as the Brookhaven Protein Database, and annealed onto the existing framework. Such a comparison is preferably accomplished by utilizing the ends of the template protein backbone, into which a loop or insert is to be added, as a pair of reference points in a search of a subset of the protein database. This search identifies known secondary structural units, of the same length as the unknown insert, which start and finish in a manner spatially similar and complementary to the reference points.

**2. Refinement Of The Model.**

The complete model is refined by fully minimizing the energy of the model of the protein with a high affinity ligand in the binding pocket. Minimization of the complete model is preferably accomplished using an algorithm such as adopted-basis set Newton-Raphson, with a dielectric constant of 1 to 20, initially holding the peptide backbone rigid (until the root mean square difference is less than 0.01), and then without any constraints. Semi-systematic refinement of the individual side chain conformations is preferably performed by manual pairing of complimentary charged residues to a known receptor ligand, followed by repeated minimization until a consistent low energy solution is attained. Pairs are preferably selected by the surface distribution of the respective complementary charged residue side chains.

**3. Calculating The Interaction Energy.**

The interaction energy ($E_{interact}$) for the individual molecules, such as basis set molecules, can be calculated as in equation 1.

$$(E_{interact} = E_{receptor+molecule} - (E_{receptor} + E_{molecule}) \quad \text{(Eq. 1)}.$$

The energy of the protein ($E_{receptor}$) and the individual molecules ($E_{molecule}$) can be calculated using standard techniques. These energies can be calculated using known techniques, based on, for example, the principles and techniques described in Kao and Allinger, *J. Am. Chem. Soc.* 99:975 (1972), and Brooks *et al.*, *J. Comp. Chem.* 4:187-217 (1983). Preferably, the energies are calculated with the aid of a molecular modeling computer program such as those described elsewhere herein. The basis set

molecules are preferably modeled in a fully ionized state. To determine the energy of a receptor/molecule complex ($E_{receptor+molecule}$), individual molecules should be placed within close proximity (2 to 3 Å) of the expected binding pocket model, followed by minimization of the receptor/molecule complex. For each molecule the starting conformation and orientation of the molecule within the binding pocket should be systematically adjusted and the complex re-minimized. Only the lowest energy structure (that is, the structure having the lowest $E_{receptor+molecule}$) should be retained after each iteration.

**4. Generating A Predictive Equation.**

The characteristics of the molecules, such as, but not limited to, volume, can be computed by, for example, employing a 0.5 Å grid overlaying the van der Waals surface of the final bound conformation of the individual molecules. Rotatable bonds for a particular molecule can be identified as those bonds whose position in the bound complex are necessarily fixed by interactions with the protein surface. Regression analysis, such as linear regression analysis, of these characteristics with the observed affinity of these ligands results in a predictive equation such as equation 2.

$$\text{Protein Affinity} = -xE_{interact} + y\text{Mol.Charc.}_{ligand} - z\text{Mol.Charc.}_{ligand} + N \quad \text{(Eq. 2)}$$

The predictive equation can use as many molecular characteristics as desired. The use of two, three, or four molecular characteristics is preferred. The use of two molecular characteristics (in addition to $E_{interact}$) is most preferred.

**5. Calculating The Interaction Energy Of A Potential Ligand.**

The interaction energy ($E_{interact}$*) for a potential ligand molecule can be calculated as in Equation 3.

$$E_{interact}^* = E_{receptor+molecule}^* - (E_{receptor} + E_{molecule}^*) \quad \text{(Eq. 3)}$$

The energy of the protein ($E_{receptor}$) and the potential ligand molecule ($E_{molecule}$*) can be calculated using standard techniques. The potential ligand molecule is preferably modeled in a fully ionized state. To

calculate $E_{receptor+molecule}$*, the potential ligand molecule should be placed within close proximity (2 to 3 Å) of the expected binding pocket model, and the receptor/molecule complex re-minimized. The conformation and orientation of the molecule within the binding pocket should then be systematically adjusted and the complex re-minimized. Only the lowest energy structure should be retained after each iteration, $E_{receptor+molecule}$*).

**6. Calculating The Affinity Of A Potential Ligand.**

The characteristics of a potential ligand molecule (the same characteristics determined and used for the basis set molecules) can be computed employing a 0.5 Å grid overlaying the van der Waals surface of the final bound conformation of the potential ligand molecule. Rotatable bonds for the potential ligand molecule can be identified as those bonds whose position in the bound complex are necessarily fixed by interactions with the protein surface. The results can then be inserted into the predictive equation (Equation 2) and the resulting affinity for the potential ligand molecule for the protein can be calculated.

**7. Predicting the Selectivity of Potential Ligands.**

Many binding proteins belong to families of binding proteins which can, to a greater or lesser extent, interact with similar ligands. Families of neurotransmitter receptors are well known examples of this. For various reasons, it is desirable to alter the activity of one or a subset of binding proteins in such a family. For this purpose, specific ligands have been discovered which have a higher affinity for one binding protein in a family than for other members. The disclosed method can be used to identify potential ligands which are selective for one or a subset of members of a binding protein family. Preferably, this is accomplished by building and refining models of the binding pockets for relevant members of a binding protein family, and generating predictive equations for each model. The affinity of a potential ligand molecule can then be calculated for each binding protein and the affinities compared. Selective ligand molecules can be identified as those having a desired pattern of affinities for the binding protein family members. For example, a ligand might be

sought having a high affinity for one of the binding proteins but not for any of the others. Such ligands could then be used for the study of the activity of the binding protein of interest, or for selectively altering the activity of the binding protein of interest.

## Examples

### Example 1: AMPA Receptor Model

The following example illustrates application of the disclosed method to the AMPA receptor GluR3.

(1) Alignment of LAOBP and GluR3 was determined in a manner similar to that suggested by Stern-Bach *et al.* with a correction for the missing lysine at position 683 of GluR3. The resulting alignment is shown in Figure 5. A topographical model of GluR3 based upon the known crystal structure of LAOBP was then constructed. The model was constructed employing the protein modeling package of "Quanta v4.0" (Molecular Simulations Incorporated). Those regions hypothesized to adopt a secondary structure topographically similar to LAOBP were modeled by duplicating those regions of the template protein (LAOBP). Conversely, those sequences of GluR3 that were additional to the basic template structure were analyzed according to the standard algorithms for predicting protein secondary structure. These sequences were subsequently modelled by comparison to a protein structural library and annealed onto the existing framework.

(2) The complete model was fully minimized using the adopted-basis set Newton-Raphson algorithm with a dielectric constant of 1, initially holding the peptide backbone rigid (until the root mean square (r.m.s.) difference was less than 0.10 Å), and then without any atomic constraints. AMPA was chosen as a representative high affinity ligand. It was manually placed in the binding pocket of the GluR3 model and minimized until the r.m.s. difference was less than 0.001 Å. Semi-systematic adjustment of the AMPA residues contacting the lining of the pocket and the individual side chain conformations was performed by

manual pairing of complementary charged residues, followed by repeated minimization until a consistent low energy solution was attained. The coordinates of the atoms in the resulting structure are listed in Table 3.

(3) The interaction energies ($E_{interact}$) for the molecules in a basis set for the AMPA receptor were calculated as in equation 1.

$$E_{interact} = E_{receptor+ligand} - (E_{receptor} + E_{ligand}) \qquad \text{(Eq. 1)}$$

The energies of the protein ($E_{receptor}$) and the individual molecules ($E_{molecule}$) were calculated using the protein modeling package "Quanta v4.0". The AMPA basis set molecules 1 to 15 (Figure 3) were modeled in a fully ionized state. Individual molecules were placed within close proximity (2 to 3 Å) of the expected binding pocket, and the receptor/molecule complex was re-minimized. For each of these antagonists, the conformation and the orientation of the molecule within the binding pocket was systematically adjusted and the complex re-minimized. Adjustments were made to both the torsional angles and the position of the molecule in the binding pocket. Only the lowest energy structure was retained after each iteration. The resulting minimum energy was used for $E_{receptor+ligand}$ in equation 1. The calculated $E_{interact}$ for each molecule in the basis set is shown in Table 1.

Table 1 - Data set for AMPA receptor basis set molecules

| Ligand | $IC_{50}$ ($^3$[H]AMPA) ($\mu$M) | $p(IC_{50})$ | $E_{interact}$ | Volume (Å$^3$) | Rot. Bonds | Predicted $p(IC_{50})$ | Residual |
|---|---|---|---|---|---|---|---|
| 1 | 0.052 | 7.28 | -232 | 234 | 1 | 7.36 | -0.08 |
| 2 | 0.080 | 7.10 | -266 | 216 | 2 | 6.44 | +0.66 |
| 3 | 1.166 | 6.78 | -271 | 245 | 2 | 6.91 | -0.13 |
| 4 | 1.153 | 6.82 | -263 | 256 | 2 | 6.94 | -0.12 |
| 5 | 0.34 | 6.47 | -216 | 170 | 1 | 6.11 | +0.36 |
| 6 | 0.20 | 6.70 | -205 | 173 | 1 | 6.24 | +0.46 |
| 7 | 2.00 | 5.70 | -220 | 151 | 1 | 6.04 | -0.34 |
| 8 | 0.15 | 6.82 | -175 | 290 | 1 | 7.23 | -0.41 |
| 9 | 0.70 | 6.15 | -155 | 250 | 1 | 6.37 | -0.22 |
| 10 | 7.20 | 5.14 | -145 | 201 | 1 | 5.55 | -0.41 |
| 11 | 0.58 | 6.24 | -194 | 257 | 2 | 5.46 | +0.78 |
| 12 | 0.63 | 6.20 | -183 | 240 | 2 | 5.55 | +0.65 |
| 13 | 1.35 | 5.87 | -190 | 238 | 2 | 5.29 | +0.58 |
| 14 | 44.0 | 4.36 | -285 | 248 | 4 | 4.75 | -0.39 |
| 15 | 24.0 | 4.62 | -225 | 179 | 2 | 5.28 | -0.66 |
| 16 | 0.85 | 6.07 | -209 | 242 | 2 | 5.90 | +0.17 |

(4) The volume of the ligands was computed employing a 0.5 Å grid overlaying the van der Waals surface of the final bound conformation of the individual ligands. Rotatable bonds for a particular ligand were assessed as those bonds whose position in the bound complex were necessarily fixed by interactions with the protein surface. Regression analysis of this data with the observed affinity of these ligands gave the relationship in equation 4, which is the predictive equation for the GluR3 model.

$$\text{GluR3 Affinity} = -0.016E_{interact} + 0.014Vol_{ligand} - 1.2Rot_{bonds} + 1.723 \quad \text{(Eq. 4)}$$

The predictive equation was used to calculate a predicted affinity for each of the basis set molecules. Measures of affinity (both actual and as calculated), volume, and the number of interacting rotatable bonds for each of the molecules in the basis set are shown in Table 1. $IC_{50}$ refers to the concentration of the indicated ligand at which half of bound AMPA is released (a measure of the relative affinities the receptor has for AMPA and the ligand). The experimentally determined measurements are reported in Bigge *et al.*, *J. Med. Chem.* 38:3720-3740 (1995), for ligands 1-4, 6, 14, and 15, in Johansen *et al.*, *Eur. J. Pharmacol.-Mol. Pharmacol. Sect.* 246:195 (1993), for ligands 5 and 10, in Ohmuri *et al.*, *J. Med. Chem.* 37:467-475 (1994), for ligand 7, in Watjen and Drwjer, PCT Application WO 94/26747, for ligand 8, in Watjen *et al.*, *Bioorg. & Med. Chem. Lett.* 4:371-376 (1994), for ligand 9, and in Arnold *et al.*, European Patent No. 93306745.6, for ligands 11-13. $p(IC_{50})$ refers to the log of $IC_{50}$. The residual represents the difference between $p(IC_{50})$ and predicted $p(IC_{50})$ for each basis set molecule.

(5) The interaction energy ($E_{interact}$*) for a potential ligand molecule, compound 16 in Figure 3, was calculated using equation 5. Compound 16 is described (as compound 7b) in Lubisch *et al.*, *Bioog. & Med. Chem. Lett.* 6:2887 (1996). The energies of the protein ($E_{receptor}$) and the potential ligand molecule ($E_{16}$) were calculated using the protein modeling package to be about -17154 and -14, respectively. The potential

ligand molecule was modeled in a fully ionized state. The molecule was placed within close proximity (2 to 3 Å) of the expected binding pocket, and the receptor/molecule complex was re-minimized. The conformation and orientation of the potential ligand molecule within the binding pocket was systematically adjusted and the complex re-minimized. Adjustments were made to both the torsional angles and the position of the molecule in the binding pocket. Only the lowest energy structure was retained after each iteration.

$$E_{interact}^* = E_{receptor+16}^* - (E_{receptor} + E_{16}^*) \qquad \text{(Eq. 5)}$$

$$= -17{,}377 - (-17{,}154 - 14)$$

$$= -209$$

(6) The volume of the potential ligand molecule was computed employing a 0.5 Å grid overlaying the van der Waals surface of the final bound conformation of the individual species. Interacting rotatable bonds for the potential ligand molecule were assessed as those bonds whose position in the bound complex were necessarily fixed by interactions with the protein surface. The rotatable bonds in compound 16 are indicated with the label R in Figure 3. The results were applied to equation 4 and the resulting affinity for protein binding was calculated. The predicted affinity (predicted $p(IC_{50})$) of 5.9 was calculated by substituting the appropriate molecular characteristics into the predictive equation (Equation 4).

$$\text{GluR3 Affinity} = -0.016E_{interact} + 0.014Vol_{ligand} - 1.2Rot_{bonds} + 1.723 \qquad \text{(Eq. 4)}$$

$$= (-0.016 \times -209) + (0.014 \times 242) - (1.2 \times 2) + 1.723$$

$$= 5.9$$

The calculated affinity ($IC_{50}$) was thus 1.25 $\mu$M. The experimentally determined affinity for compound 16 is 0.85 $\mu$M.

**Example 2: Kainate Receptor Model**

The following example illustrates application of the disclosed method to the kainate receptor GluR6.

(1) Alignment of LAOBP and GluR6 was determined in a manner similar to that suggested by Stern-Bach *et al.* The resulting alignment is shown in Figure 5. A topographical model of GluR6 based upon the known crystal structure of LAOBP was then constructed. The model was constructed employing the protein modeling package of "Quanta v4.0" (Molecular Simulations Incorporated). Those regions hypothesized to adopt a secondary structure topographically similar to LAOBP were modelled by duplicating those regions of the template protein (LAOBP). Conversely, those sequences of GluR6 that were additional to the basic template structure were analyzed according to the standard algorithms for predicting protein secondary structure. These sequences were subsequently modelled by comparison to a protein structural library and annealed onto the existing framework.

(2) The complete model was fully minimized using the adopted-basis set Newton-Raphson algorithm with a dielectric constant of 1, initially holding the peptide backbone rigid (until the r.m.s. difference was less than 0.01 Å), and then without any atomic constraints. Kainic acid was chosen as a representative high affinity ligand. It was manually placed in the binding pocket of the GluR6 model and minimized until the r.m.s. difference was less than 0.001 Å. Semi-systematic adjustment of the KA residues contacting the lining of the pocket and the individual side chain conformations was performed by manual pairing of complimentary charged residues, followed by repeated minimization until a consistent low energy solution was attained. The coordinates of the atoms in the resulting structure are listed in Table 4.

(3) The interaction energies ($E_{interact}$) for the molecules in a basis set for the KA receptor were calculated as in equation 1.

$$E_{interact} = E_{receptor+ligand} - (E_{receptor} + E_{ligand}) \quad \text{(Eq. 1)}$$

The energies of the protein ($E_{receptor}$) and the individual molecules ($E_{molecule}$) were calculated using the protein modeling package "Quanta v4.0". Members of the KA receptor basis set were chosen to reflect the natural ligands of these receptors and the most potent of synthetic ligands. The

individual members of the basis set, compounds 1-10 in Figure 4. The basis set molecules were modeled in a fully ionized state. Individual molecules were placed within close proximity (2 to 3 Å) of the expected binding pocket and the receptor/molecule complex was re-minimized. For each of these antagonists, the conformation and orientation of the molecule within the binding pocket was systematically adjusted and the complex re-minimized. Only the lowest energy structure was retained after each iteration. Each ligand was also fully minimized in the absence of the receptor model. Additionally, a conformational analysis of each of the ligands was performed in order to estimate the conformational flexibility of each species. Earlier work had suggested that while the *threo*-4-alkyl glutamates were conformationally mobile in aqueous solution at room temperature, the backbone $^1H$-$^1H$ coupling constants suggested that rotation around the $C_3$-$C_4$ bond was considerably retarded. Thus, each of the *erythro* ligands was assigned one less rotatable bond than its *threo* counterpart. Kainic acid was assigned two rotatable bonds on the basis of free rotation around the pseudo $C_3$-$C_4$ bond and free rotation of the isopropenyl side chain. The resulting minimum energy was used for $E_{receptor+ligand}$ in equation 1. The $E_{interact}$ for each molecule in the basis set is shown in Table 2.

Table 2 - KA receptor model basis set data

| Ligand | $IC_{50}$($^3$[H]KA) ($\mu$M) | p($IC_{50}$) | $E_{interact}$ | Rot. Bonds | Predicted (p($IC_{50}$) | Residual |
|---|---|---|---|---|---|---|
| 1: L-Glu | 0.42 | 6.38 | -137.2 | 2 | 6.14 | +0.24 |
| 2: kainic | 0.020 | 7.70 | -146.1 | 2 | 7.25 | +0.45 |
| 3: 2081 | 0.045 | 7.46 | -135.5 | 1 | 6.89 | +0.46 |
| 4: 2048 | 3.00 | 5.52 | -130.9 | 2 | 5.36 | +0.16 |
| 5: 2077 | 1.34 | 5.87 | -134.5 | 1 | 6.77 | -0.90 |
| 6: 2047 | 3.00 | 5.52 | -135.0 | 2 | 5.87 | -0.33 |
| 7: 2084 | 2.80 | 5.55 | -133.8 | 2 | 5.72 | -0.18 |
| 8: 2072 | 20.0 | 4.70 | -136.9 | 3 | 5.14 | -0.44 |
| 9: 2194 | 32.0 | 4.50 | -125.0 | 2 | 4.62 | -0.12 |
| 10: 2139 | 100 | 4.00 | -120.3 | 2 | 4.03 | -0.03 |
| 11: 2114 | 300 | 3.50 | -115.4 | 2 | 3.42 | +0.08 |
| 12: 2116 | 3.10 | 5.51 | -127.1 | 2 | 4.88 | +0.63 |
| 13: 2083 | 1.51 | 5.82 | -144.4 | 3 | 6.10 | -0.28 |

(4) The volume of the ligands was computed employing a 0.5 Å grid overlaying the van der Waals surface of the final bound conformation of the individual species. Regression analysis of this data with the observed affinity of these ligands gives the relationship in equation 6, which is the predictive equation for the GluR6 model.

$$\text{GluR6 Affinity} = -0.125E_{interact} - 0.963Rot_{bonds} - 9.063 \quad \text{(Eq. 6)}$$

The predictive equation was used to calculate a predicted affinity for each of the basis set molecules. Measures of affinity (both actual and as calculated), volume, and the number of interacting rotatable bonds for each of the molecules in the basis set are shown in Table 2.

(5) The interaction energy ($E_{interact\ (SYM\ 2083)}$) for SYM 2083, shown as compound 3 in Figure 4, was calculated as in Equation 7. The energies of the protein ($E_{receptor}$) and SYM 2083 ($E_{SYM\ 2083}$) were calculated using the protein modeling package. The novel molecule SYM 2083 was modeled in a fully ionized state. SYM 2083 was placed within close proximity (2 to 3 Å) of the expected binding pocket, and the receptor/SYM 2083 complex was re-minimized. The conformation and orientation of SYM 2083 within the binding pocket was systematically adjusted and the complex re-minimized. Only the lowest energy structure was retained after each iteration.

$$E_{interact\ (SYM\ 2083)} = E_{receptor+\ SYM\ 2083} - (E_{receptor} + E_{SYM\ 2083}) \quad \text{(Eq. 7)}$$

(6) The volume of SYM 2083 was computed employing a 0.5 Å grid overlaying the van deer Waals surface of the final bound conformation of the individual species. Rotatable bonds for SYM 2083 were assessed as those bonds whose position in the bound complex were necessarily fixed by interactions with the protein surface. The results were inserted into equation 6 and the resulting affinity for protein binding calculated. The calculated affinity ($p(IC_{50})$) was 6.10 and the experimentally determined affinity ($p(IC_{50})$) was 5.82.

**Example 3: NMDA Receptor Glutamate Site**

The following example illustrates application of the disclosed method to a glutamate site on an NMDA receptor.

(1) Alignment of LAOBP and the NMDA receptor NR2-B was determined in a manner similar to that suggested by Stern-Bach *et al.* The resulting alignment is shown in Figure 5. A topographical model based upon the known crystal structure of LAOBP was then constructed. The model was constructed employing the protein modeling package of "Quanta v4.0" (Molecular Simulations Incorporated). Those regions hypothesized to adopt a secondary structure homologous to LAOBP were modeled by duplicating those regions of the template protein. Conversely, those sequences of NR2-B that were additional to the basic template structure were analyzed according to the standard algorithms for predicting protein secondary structure. These sequences were subsequently modeled by comparison to a protein structural library and annealed onto the existing framework.

(2) The complete model was fully minimized using the adopted-basis set Newton-Raphson algorithm at a dielectric constant of 1, initially holding the peptide backbone rigid (until r.m.s. difference was less than 0.01 Å), and then without any atomic constraints. L-glutamate was chosen as a representative high affinity ligand. It was manually placed in the binding pocket of the NR2-B model and minimized until the r.m.s. was less than 0.001 Å. Semi-systematic adjustment of the L-glutamate residues contacting the lining of the pocket and the individual side chain conformations was performed by manual pairing of the charged residues, followed by repeated minimization until a consistent low energy solution was attained. The coordinates of the atoms in the resulting structure are listed in Table 5.

(3) The interaction energies ($E_{interact}$) for the individual molecules can be calculated as in equation 1. The energies of the protein ($E_{receptor}$) and the individual molecules ($E_{molecule}$) can be calculated using the protein modeling package "Quanta v4.0". Members of the NR2 receptor basis set are chosen to reflect the natural ligands of these receptors and the most potent of our initial synthetic ligands. The individual members of the basis set can be primarily chosen in order to expand the range of ligands

covered by this approach and to aid in the design of novel ligands. The basis set of molecules can be modeled in a fully ionized state. Individual molecules can be placed within close proximity (2 to 3 Å) of the expected binding pocket, and the receptor/molecule complex re-minimized. For each basis set molecule the conformation and orientation of the molecule within the binding pocket can be systematically adjusted and the complex re-minimized. Only the lowest energy structure is retained. The resulting minimum energy can be used for $E_{receptor+ligand}$ in equation 1.

$$E_{interact} = E_{receptor+molecule} - (E_{receptor} + E_{molecule}) \quad \text{(Eq. 1)}$$

(4) The volume of the ligands can be computed employing a 0.5 Å grid overlaying the van der Waals surface of the final bound conformation of the individual species. Regression of this data with the observed affinity of these ligands will give a predictive equation for the NR2 model (Equation 8).

$$\text{NR2 Affinity} = -xE_{interact} + yVol_{ligand} - zRot_{bonds} + N \quad \text{(Eq. 8)}$$

(5) The interaction energy ($E_{interact}$*) for a potential ligand molecule can calculated as in Equation 3.

$$E_{interact}^* = E_{receptor+molecule} - (E_{receptor} + E_{molecule}^*) \quad \text{(Eq. 3)}$$

The energies of the protein ($E_{receptor}$) and the potential ligand molecule ($E_{molecule}$*) can be calculated using the protein modeling package. The potential ligand molecule can be modeled in a fully ionized state, placed within close proximity (2 to 3 Å) of the expected binding pocket, and the receptor/molecule complex re-minimized. The conformation and orientation within the binding pocket can be systematically adjusted and the complex re-minimized. Only the lowest energy structure is retained after each iteration.

(6) The volume of the potential ligand molecule is computed employing a 0.5 Å grid overlaying the van der Waals surface of the final bound conformation of the individual species. Rotatable bonds for the potential ligand molecule are assessed as those bonds whose position in the bound complex were necessarily fixed by interactions with the protein

surface. The results are inserted into the predictive equation (Equation 8) and the resulting affinity for protein binding calculated.

**Example 4: NMDA Receptor Glycine Site**

The following example illustrates application of the disclosed method to a glycine site on an NMDA receptor.

(1) Alignment of LAOBP and the NMDA receptor NR1 was determined in a manner similar to that suggested by Stern-Bach *et al.* The resulting alignment is shown in Figure 5. A topographical model based upon the known crystal structure of LAOBP was then constructed. The model was constructed employing the protein modeling package of "Quanta v4.0" (Molecular Simulations Incorporated). Those regions hypothesized to adopt a secondary structure homologous to LAOBP were modeled by duplicating those regions of the template protein. Conversely, those sequences of NR1 that were additional to the basic template structure were analyzed according to the standard algorithms for predicting protein secondary structure. These sequences were subsequently modeled by comparison to a protein structural library and annealed onto the existing framework.

(2) The complete model was fully minimized using the adopted-basis set Newton-Raphson algorithm at a dielectric constant of 1, initially holding the peptide backbone rigid (until r.m.s. difference was less than 0.01 Å), and then without any atomic constraints. L-glycine was chosen as a representative high affinity ligand. It was manually placed in the binding pocket of the NR1 model and minimized until the r.m.s. was less than 0.001 Å. Semi-systematic adjustment of the glycine residues contacting the lining of the pocket and the individual side chain conformations was performed by manual pairing of the charged residues, followed by repeated minimization until a consistent low energy solution was attained. The coordinates of the atoms in the resulting structure are listed in Table 6.

(3) The interaction energies ($E_{interact}$) for the individual molecules can be calculated as in equation 1. The energies of the protein ($E_{receptor}$)

and the individual molecules ($E_{molecule}$) can be calculated using the protein modeling package "Quanta v4.0". Members of the NR1 receptor basis set can be chosen to reflect the natural ligands of these receptors and the most potent of our initial synthetic ligands. The individual members of the basis set can be primarily chosen in order to expand the range of ligands covered by this approach and to aid in the design of novel ligands. The basis set of molecules are modeled in a fully ionized state. Individual molecules can be placed within close proximity (2 to 3 Å) of the expected binding pocket, and the receptor/molecule complex re-minimized. For each ligand the conformation and orientation of the molecule within the binding pocket can be systematically adjusted and the complex re-minimized. Only the lowest energy structure is retained. The resulting minimum energy is used for $E_{receptor+ligand}$ in equation 1.

$$E_{interact} = E_{receptor+molecule} - (E_{receptor} + E_{molecule}) \quad \text{(Eq. 1)}$$

(4) The volume of the ligands can be computed employing a 0.5 Å grid overlaying the van der Waals surface of the final bound conformation of the individual species. Regression of this data with the observed affinity of these ligands will give a predictive equation for the NR1 model (Equation 9).

$$\text{NR1 Affinity} = -xE_{interact} + yVol_{ligand} - zRot_{bonds} + N \quad \text{(Eq. 9)}$$

(5) The interaction energy ($E_{interact}$*) for the potential ligand molecule can be calculated as in Equation 3.

$$E_{interact}^* = E_{receptor+molecule} - (E_{receptor} + E_{molecule}^*) \quad \text{(Eq. 3)}$$

The energies of the protein ($E_{receptor}$) and the potential ligand molecule ($E_{molecule}$*) can be calculated using the protein modeling package. The potential ligand molecule can be modeled in a fully ionized state, placed within close proximity (2 to 3 Å) of the expected binding pocket, and the receptor/molecule complex re-minimized. The conformation and orientation within the binding pocket can be systematically adjusted and the complex re-minimized. Only the lowest energy structure is retained after each iteration.

(6) The volume of the potential ligand molecule can be computed employing a 0.5 Å grid overlaying the van der Waals surface of the final bound conformation of the individual species. Rotatable bonds for the potential ligand molecule are assessed as those bonds whose position in the bound complex were necessarily fixed by interactions with the protein surface. The results can be inserted into the predictive equation (Equation 9) and the resulting affinity for protein binding calculated.

**Binding Protein Model Coordinates**

Coordinates of atoms in the computer models of the AMPA receptor GluR3, the NMDA receptor NR2-B, the kainate receptor GluR6, and the NMDA receptor NR1 built and revised using the disclosed method are shown in Tables 3 through 6. Table 3 shows the coordinates of 2706 atoms in the model of the AMPA receptor GluR3. Table 4 shows the coordinates of 2700 atoms in the model of the kainate receptor GluR6. Table 5 shows the coordinates of 2653 atoms in the model of the NMDA receptor NR2-B. Table 6 shows the coordinates of 2975 atoms in the model of the NMDA receptor NR1.

**TABLE 3**

REMARK 1 AMPA Receptor (GluR3) Model of the Glutamate Binding Site

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1 | N | GLY | 2 | 260 | 27.989 | 84.331 | 28.873 | 1.00 | 0.00 |
| ATOM | 2 | CA | GLY | 2 | 260 | 29.091 | 83.371 | 28.965 | 1.00 | 0.00 |
| ATOM | 3 | C | GLY | 2 | 260 | 28.491 | 82.067 | 29.445 | 1.00 | 0.00 |
| ATOM | 4 | O | GLY | 2 | 260 | 27.382 | 81.718 | 29.054 | 1.00 | 0.00 |
| ATOM | 5 | 1HT | GLY | 2 | 260 | 28.083 | 85.110 | 29.561 | 1.00 | 0.00 |
| ATOM | 6 | 2HT | GLY | 2 | 260 | 27.094 | 83.844 | 29.099 | 1.00 | 0.00 |
| ATOM | 7 | 3HT | GLY | 2 | 260 | 27.938 | 84.794 | 27.947 | 1.00 | 0.00 |
| ATOM | 8 | N | VAL | 2 | 261 | 29.222 | 81.400 | 30.348 | 1.00 | 0.00 |
| ATOM | 9 | CA | VAL | 2 | 261 | 28.576 | 80.292 | 31.059 | 1.00 | 0.00 |
| ATOM | 10 | C | VAL | 2 | 261 | 28.143 | 80.710 | 32.466 | 1.00 | 0.00 |
| ATOM | 11 | O | VAL | 2 | 261 | 28.347 | 80.077 | 33.497 | 1.00 | 0.00 |
| ATOM | 12 | CB | VAL | 2 | 261 | 29.469 | 79.034 | 31.008 | 1.00 | 0.00 |
| ATOM | 13 | CG1 | VAL | 2 | 261 | 30.809 | 79.223 | 31.728 | 1.00 | 0.00 |
| ATOM | 14 | CG2 | VAL | 2 | 261 | 28.707 | 77.771 | 31.425 | 1.00 | 0.00 |
| ATOM | 15 | H | VAL | 2 | 261 | 30.126 | 81.727 | 30.628 | 1.00 | 0.00 |
| ATOM | 16 | N | GLU | 2 | 262 | 27.530 | 81.889 | 32.465 | 1.00 | 0.00 |
| ATOM | 17 | CA | GLU | 2 | 262 | 27.238 | 82.527 | 33.745 | 1.00 | 0.00 |
| ATOM | 18 | C | GLU | 2 | 262 | 25.883 | 82.158 | 34.305 | 1.00 | 0.00 |
| ATOM | 19 | O | GLU | 2 | 262 | 25.753 | 81.831 | 35.482 | 1.00 | 0.00 |
| ATOM | 20 | CB | GLU | 2 | 262 | 27.426 | 84.053 | 33.689 | 1.00 | 0.00 |
| ATOM | 21 | CG | GLU | 2 | 262 | 27.442 | 84.702 | 32.297 | 1.00 | 0.00 |
| ATOM | 22 | CD | GLU | 2 | 262 | 26.143 | 84.434 | 31.564 | 1.00 | 0.00 |
| ATOM | 23 | OE1 | GLU | 2 | 262 | 26.123 | 83.642 | 30.637 | 1.00 | 0.00 |
| ATOM | 24 | OE2 | GLU | 2 | 262 | 25.132 | 85.008 | 31.910 | 1.00 | 0.00 |
| ATOM | 25 | H | GLU | 2 | 262 | 27.074 | 82.138 | 31.612 | 1.00 | 0.00 |
| ATOM | 26 | N | ARG | 2 | 263 | 24.894 | 82.182 | 33.391 | 1.00 | 0.00 |
| ATOM | 27 | CA | ARG | 2 | 263 | 23.498 | 81.858 | 33.695 | 1.00 | 0.00 |
| ATOM | 28 | C | ARG | 2 | 263 | 23.277 | 80.850 | 34.820 | 1.00 | 0.00 |
| ATOM | 29 | O | ARG | 2 | 263 | 23.477 | 79.643 | 34.709 | 1.00 | 0.00 |
| ATOM | 30 | CB | ARG | 2 | 263 | 22.740 | 81.521 | 32.395 | 1.00 | 0.00 |
| ATOM | 31 | CG | ARG | 2 | 263 | 22.960 | 80.159 | 31.712 | 1.00 | 0.00 |
| ATOM | 32 | CD | ARG | 2 | 263 | 24.354 | 79.834 | 31.157 | 1.00 | 0.00 |
| ATOM | 33 | NE | ARG | 2 | 263 | 24.355 | 78.468 | 30.622 | 1.00 | 0.00 |
| ATOM | 34 | CZ | ARG | 2 | 263 | 24.867 | 78.167 | 29.408 | 1.00 | 0.00 |
| ATOM | 35 | NH1 | ARG | 2 | 263 | 25.548 | 79.078 | 28.724 | 1.00 | 0.00 |
| ATOM | 36 | NH2 | ARG | 2 | 263 | 24.675 | 76.964 | 28.886 | 1.00 | 0.00 |
| ATOM | 37 | H | ARG | 2 | 263 | 25.139 | 82.516 | 32.482 | 1.00 | 0.00 |
| ATOM | 38 | HE | ARG | 2 | 263 | 23.895 | 77.751 | 31.159 | 1.00 | 0.00 |
| ATOM | 39 | 1HH1 | ARG | 2 | 263 | 25.934 | 78.837 | 27.832 | 1.00 | 0.00 |
| ATOM | 40 | 2HH1 | ARG | 2 | 263 | 25.713 | 80.009 | 29.066 | 1.00 | 0.00 |
| ATOM | 41 | 1HH2 | ARG | 2 | 263 | 24.923 | 76.804 | 27.930 | 1.00 | 0.00 |
| ATOM | 42 | 2HH2 | ARG | 2 | 263 | 24.273 | 76.220 | 29.420 | 1.00 | 0.00 |
| ATOM | 43 | N | MET | 2 | 264 | 22.927 | 81.435 | 35.975 | 1.00 | 0.00 |
| ATOM | 44 | CA | MET | 2 | 264 | 23.177 | 80.656 | 37.187 | 1.00 | 0.00 |
| ATOM | 45 | C | MET | 2 | 264 | 22.253 | 79.480 | 37.450 | 1.00 | 0.00 |
| ATOM | 46 | O | MET | 2 | 264 | 21.036 | 79.608 | 37.534 | 1.00 | 0.00 |
| ATOM | 47 | CB | MET | 2 | 264 | 23.255 | 81.562 | 38.422 | 1.00 | 0.00 |
| ATOM | 48 | CG | MET | 2 | 264 | 21.985 | 82.370 | 38.709 | 1.00 | 0.00 |
| ATOM | 49 | SD | MET | 2 | 264 | 21.993 | 83.112 | 40.347 | 1.00 | 0.00 |
| ATOM | 50 | CE | MET | 2 | 264 | 21.960 | 81.587 | 41.306 | 1.00 | 0.00 |
| ATOM | 51 | H | MET | 2 | 264 | 22.725 | 82.417 | 35.964 | 1.00 | 0.00 |
| ATOM | 52 | N | GLU | 2 | 265 | 22.901 | 78.329 | 37.619 | 1.00 | 0.00 |
| ATOM | 53 | CA | GLU | 2 | 265 | 22.245 | 77.239 | 38.335 | 1.00 | 0.00 |
| ATOM | 54 | C | GLU | 2 | 265 | 22.798 | 77.230 | 39.745 | 1.00 | 0.00 |
| ATOM | 55 | O | GLU | 2 | 265 | 23.853 | 77.833 | 39.953 | 1.00 | 0.00 |
| ATOM | 56 | CB | GLU | 2 | 265 | 22.527 | 75.955 | 37.573 | 1.00 | 0.00 |
| ATOM | 57 | CG | GLU | 2 | 265 | 21.334 | 75.540 | 36.713 | 1.00 | 0.00 |
| ATOM | 58 | CD | GLU | 2 | 265 | 20.328 | 74.721 | 37.509 | 1.00 | 0.00 |
| ATOM | 59 | OE1 | GLU | 2 | 265 | 19.614 | 73.922 | 36.929 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 60 | OE2 | GLU | 2 | 265 | 20.259 | 74.816 | 38.727 | 1.00 | 0.00 |
| ATOM | 61 | H | GLU | 2 | 265 | 23.866 | 78.309 | 37.360 | 1.00 | 0.00 |
| ATOM | 62 | N | SER | 2 | 266 | 22.808 | 76.595 | 40.690 | 1.00 | 0.00 |
| ATOM | 63 | CA | SER | 2 | 266 | 22.270 | 76.930 | 42.105 | 1.00 | 0.00 |
| ATOM | 64 | C | SER | 2 | 266 | 23.527 | 76.384 | 42.855 | 1.00 | 0.00 |
| ATOM | 65 | O | SER | 2 | 266 | 24.537 | 77.069 | 42.732 | 1.00 | 0.00 |
| ATOM | 66 | CB | SER | 2 | 266 | 20.862 | 76.873 | 42.725 | 1.00 | 0.00 |
| ATOM | 67 | OG | SER | 2 | 266 | 20.151 | 75.774 | 42.128 | 1.00 | 0.00 |
| ATOM | 68 | H | SER | 2 | 266 | 21.292 | 76.055 | 40.376 | 1.00 | 0.00 |
| ATOM | 69 | HG | SER | 2 | 266 | 19.462 | 76.058 | 41.576 | 1.00 | 0.00 |
| ATOM | 70 | N | PRO | 2 | 267 | 23.544 | 75.217 | 43.578 | 1.00 | 0.00 |
| ATOM | 71 | CA | PRO | 2 | 267 | 24.854 | 74.718 | 44.064 | 1.00 | 0.00 |
| ATOM | 72 | C | PRO | 2 | 267 | 25.897 | 74.459 | 42.972 | 1.00 | 0.00 |
| ATOM | 73 | O | PRO | 2 | 267 | 25.652 | 74.714 | 41.795 | 1.00 | 0.00 |
| ATOM | 74 | CB | PRO | 2 | 267 | 24.489 | 73.418 | 44.784 | 1.00 | 0.00 |
| ATOM | 75 | CG | PRO | 2 | 267 | 23.030 | 73.561 | 45.189 | 1.00 | 0.00 |
| ATOM | 76 | CD | PRO | 2 | 267 | 22.459 | 74.347 | 44.025 | 1.00 | 0.00 |
| ATOM | 77 | N | ILE | 2 | 268 | 27.061 | 73.905 | 43.376 | 1.00 | 0.00 |
| ATOM | 78 | CA | ILE | 2 | 268 | 28.146 | 73.483 | 42.471 | 1.00 | 0.00 |
| ATOM | 79 | C | ILE | 2 | 268 | 28.877 | 72.309 | 43.140 | 1.00 | 0.00 |
| ATOM | 80 | O | ILE | 2 | 268 | 28.428 | 71.879 | 44.204 | 1.00 | 0.00 |
| ATOM | 81 | CB | ILE | 2 | 268 | 29.041 | 74.711 | 42.174 | 1.00 | 0.00 |
| ATOM | 82 | CG1 | ILE | 2 | 268 | 30.059 | 74.523 | 41.040 | 1.00 | 0.00 |
| ATOM | 83 | CG2 | ILE | 2 | 268 | 29.712 | 75.225 | 43.454 | 1.00 | 0.00 |
| ATOM | 84 | CD1 | ILE | 2 | 268 | 30.824 | 75.800 | 40.690 | 1.00 | 0.00 |
| ATOM | 85 | H | ILE | 2 | 268 | 27.202 | 73.726 | 44.354 | 1.00 | 0.00 |
| ATOM | 86 | N | GLU | 2 | 269 | 29.975 | 71.782 | 42.565 | 1.00 | 0.00 |
| ATOM | 87 | CA | GLU | 2 | 269 | 30.814 | 70.919 | 43.391 | 1.00 | 0.00 |
| ATOM | 88 | C | GLU | 2 | 269 | 32.294 | 71.268 | 43.306 | 1.00 | 0.00 |
| ATOM | 89 | O | GLU | 2 | 269 | 33.058 | 70.684 | 42.539 | 1.00 | 0.00 |
| ATOM | 90 | CB | GLU | 2 | 269 | 30.577 | 69.433 | 43.083 | 1.00 | 0.00 |
| ATOM | 91 | CG | GLU | 2 | 269 | 31.019 | 68.539 | 44.250 | 1.00 | 0.00 |
| ATOM | 92 | CD | GLU | 2 | 269 | 30.916 | 67.061 | 43.913 | 1.00 | 0.00 |
| ATOM | 93 | OE1 | GLU | 2 | 269 | 29.896 | 66.604 | 43.423 | 1.00 | 0.00 |
| ATOM | 94 | OE2 | GLU | 2 | 269 | 31.866 | 66.333 | 44.150 | 1.00 | 0.00 |
| ATOM | 95 | H | GLU | 2 | 269 | 30.258 | 72.005 | 41.634 | 1.00 | 0.00 |
| ATOM | 96 | N | SER | 2 | 270 | 32.690 | 72.248 | 44.138 | 1.00 | 0.00 |
| ATOM | 97 | CA | SER | 2 | 270 | 34.124 | 72.348 | 44.436 | 1.00 | 0.00 |
| ATOM | 98 | C | SER | 2 | 270 | 34.498 | 71.263 | 45.447 | 1.00 | 0.00 |
| ATOM | 99 | O | SER | 2 | 270 | 33.771 | 70.281 | 45.590 | 1.00 | 0.00 |
| ATOM | 100 | CB | SER | 2 | 270 | 34.480 | 73.772 | 44.896 | 1.00 | 0.00 |
| ATOM | 101 | OG | SER | 2 | 270 | 35.875 | 74.054 | 44.661 | 1.00 | 0.00 |
| ATOM | 102 | H | SER | 2 | 270 | 31.985 | 72.651 | 44.728 | 1.00 | 0.00 |
| ATOM | 103 | HG | SER | 2 | 270 | 35.942 | 74.210 | 43.722 | 1.00 | 0.00 |
| ATOM | 104 | N | ALA | 2 | 271 | 35.619 | 71.442 | 46.162 | 1.00 | 0.00 |
| ATOM | 105 | CA | ALA | 2 | 271 | 35.890 | 70.381 | 47.135 | 1.00 | 0.00 |
| ATOM | 106 | C | ALA | 2 | 271 | 34.803 | 70.275 | 48.204 | 1.00 | 0.00 |
| ATOM | 107 | O | ALA | 2 | 271 | 34.192 | 69.238 | 48.444 | 1.00 | 0.00 |
| ATOM | 108 | CB | ALA | 2 | 271 | 37.250 | 70.596 | 47.803 | 1.00 | 0.00 |
| ATOM | 109 | H | ALA | 2 | 271 | 36.176 | 72.271 | 46.077 | 1.00 | 0.00 |
| ATOM | 110 | N | GLU | 2 | 272 | 34.610 | 71.439 | 48.827 | 1.00 | 0.00 |
| ATOM | 111 | CA | GLU | 2 | 272 | 33.845 | 71.483 | 50.066 | 1.00 | 0.00 |
| ATOM | 112 | C | GLU | 2 | 272 | 32.335 | 71.544 | 49.939 | 1.00 | 0.00 |
| ATOM | 113 | O | GLU | 2 | 272 | 31.620 | 71.268 | 50.891 | 1.00 | 0.00 |
| ATOM | 114 | CB | GLU | 2 | 272 | 34.390 | 72.588 | 80.985 | 1.00 | 0.00 |
| ATOM | 115 | CG | GLU | 2 | 272 | 34.956 | 73.839 | 50.288 | 1.00 | 0.00 |
| ATOM | 116 | CD | GLU | 2 | 272 | 33.873 | 74.606 | 49.557 | 1.00 | 0.00 |
| ATOM | 117 | OE1 | GLU | 2 | 272 | 33.401 | 75.602 | 50.087 | 1.00 | 0.00 |
| ATOM | 118 | OE2 | GLU | 2 | 272 | 33.466 | 74.225 | 48.460 | 1.00 | 0.00 |
| ATOM | 119 | H | GLU | 2 | 272 | 34.916 | 72.287 | 48.392 | 1.00 | 0.00 |
| ATOM | 120 | N | ASP | 2 | 273 | 31.849 | 71.872 | 48.733 | 1.00 | 0.00 |
| ATOM | 121 | CA | ASP | 2 | 273 | 30.392 | 71.945 | 48.549 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 122 | C | ASP | 2 | 273 | 29.550 | 70.796 | 49.096 | 1.00 | 0.00 |
| ATOM | 123 | O | ASP | 2 | 273 | 28.420 | 70.959 | 49.553 | 1.00 | 0.00 |
| ATOM | 124 | CB | ASP | 2 | 273 | 30.041 | 72.189 | 47.078 | 1.00 | 0.00 |
| ATOM | 125 | CG | ASP | 2 | 273 | 30.263 | 73.646 | 46.719 | 1.00 | 0.00 |
| ATOM | 126 | OD1 | ASP | 2 | 273 | 31.299 | 73.987 | 46.162 | 1.00 | 0.00 |
| ATOM | 127 | OD2 | ASP | 2 | 273 | 29.415 | 74.479 | 47.011 | 1.00 | 0.00 |
| ATOM | 128 | H | ASP | 2 | 273 | 32.482 | 72.373 | 48.144 | 1.00 | 0.00 |
| ATOM | 129 | N | LEU | 2 | 274 | 30.126 | 69.581 | 49.013 | 1.00 | 0.00 |
| ATOM | 130 | CA | LEU | 2 | 274 | 29.339 | 68.439 | 49.499 | 1.00 | 0.00 |
| ATOM | 131 | C | LEU | 2 | 274 | 29.259 | 68.314 | 51.010 | 1.00 | 0.00 |
| ATOM | 132 | O | LEU | 2 | 274 | 28.386 | 67.661 | 51.586 | 1.00 | 0.00 |
| ATOM | 133 | CB | LEU | 2 | 274 | 29.806 | 67.116 | 48.904 | 1.00 | 0.00 |
| ATOM | 134 | CG | LEU | 2 | 274 | 29.570 | 66.957 | 47.405 | 1.00 | 0.00 |
| ATOM | 135 | CD1 | LEU | 2 | 274 | 30.022 | 65.576 | 46.940 | 1.00 | 0.00 |
| ATOM | 136 | CD2 | LEU | 2 | 274 | 28.122 | 67.223 | 46.999 | 1.00 | 0.00 |
| ATOM | 137 | H | LEU | 2 | 274 | 31.110 | 59.509 | 48.840 | 1.00 | 0.00 |
| ATOM | 138 | N | ALA | 2 | 275 | 30.193 | 69.024 | 51.652 | 1.00 | 0.00 |
| ATOM | 139 | CA | ALA | 2 | 275 | 29.824 | 69.388 | 53.032 | 1.00 | 0.00 |
| ATOM | 140 | C | ALA | 2 | 275 | 28.951 | 70.554 | 53.158 | 1.00 | 0.00 |
| ATOM | 141 | O | ALA | 2 | 275 | 27.887 | 70.431 | 53.776 | 1.00 | 0.00 |
| ATOM | 142 | CB | ALA | 2 | 275 | 31.227 | 69.699 | 53.774 | 1.00 | 0.00 |
| ATOM | 143 | H | ALA | 2 | 275 | 30.957 | 69.441 | 51.153 | 1.00 | 0.00 |
| ATOM | 144 | N | LYS | 2 | 276 | 29.388 | 71.682 | 52.567 | 1.00 | 0.00 |
| ATOM | 145 | CA | LYS | 2 | 276 | 28.917 | 73.011 | 52.965 | 1.00 | 0.00 |
| ATOM | 146 | C | LYS | 2 | 276 | 27.572 | 73.501 | 52.470 | 1.00 | 0.00 |
| ATOM | 147 | O | LYS | 2 | 276 | 26.882 | 74.266 | 53.143 | 1.00 | 0.00 |
| ATOM | 148 | CB | LYS | 2 | 276 | 30.016 | 74.083 | 52.767 | 1.00 | 0.00 |
| ATOM | 149 | CG | LYS | 2 | 276 | 30.565 | 74.479 | 51.375 | 1.00 | 0.00 |
| ATOM | 150 | CD | LYS | 2 | 276 | 29.653 | 75.293 | 50.438 | 1.00 | 0.00 |
| ATOM | 151 | CE | LYS | 2 | 276 | 30.361 | 76.324 | 49.529 | 1.00 | 0.00 |
| ATOM | 152 | NZ | LYS | 2 | 276 | 31.329 | 75.732 | 48.594 | 1.00 | 0.00 |
| ATOM | 153 | H | LYS | 2 | 276 | 30.169 | 71.575 | 51.953 | 1.00 | 0.00 |
| ATOM | 154 | 1HZ | LYS | 2 | 276 | 31.965 | 75.061 | 49.077 | 1.00 | 0.00 |
| ATOM | 155 | 2HZ | LYS | 2 | 276 | 30.902 | 75.230 | 47.792 | 1.00 | 0.00 |
| ATOM | 156 | 3HZ | LYS | 2 | 276 | 31.995 | 76.440 | 48.234 | 1.00 | 0.00 |
| ATOM | 157 | N | GLN | 2 | 277 | 27.207 | 73.065 | 51.255 | 1.00 | 0.00 |
| ATOM | 158 | CA | GLN | 2 | 277 | 25.881 | 73.478 | 50.796 | 1.00 | 0.00 |
| ATOM | 159 | C | GLN | 2 | 277 | 24.785 | 72.689 | 51.490 | 1.00 | 0.00 |
| ATOM | 160 | O | GLN | 2 | 277 | 24.409 | 71.601 | 51.067 | 1.00 | 0.00 |
| ATOM | 161 | CB | GLN | 2 | 277 | 25.780 | 73.382 | 49.270 | 1.00 | 0.00 |
| ATOM | 162 | CG | GLN | 2 | 277 | 24.403 | 73.689 | 48.657 | 1.00 | 0.00 |
| ATOM | 163 | CD | GLN | 2 | 277 | 24.124 | 75.176 | 48.554 | 1.00 | 0.00 |
| ATOM | 164 | OE1 | GLN | 2 | 277 | 23.176 | 75.717 | 49.124 | 1.00 | 0.00 |
| ATOM | 165 | NE2 | GLN | 2 | 277 | 24.965 | 75.821 | 47.738 | 1.00 | 0.00 |
| ATOM | 166 | H | GLN | 2 | 277 | 27.745 | 72.361 | 50.781 | 1.00 | 0.00 |
| ATOM | 167 | 1HE2 | GLN | 2 | 277 | 24.935 | 76.811 | 47.611 | 1.00 | 0.00 |
| ATOM | 168 | 2HE2 | GLN | 2 | 277 | 25.644 | 75.302 | 47.218 | 1.00 | 0.00 |
| ATOM | 169 | N | THR | 2 | 278 | 24.295 | 73.316 | 525.569 | 1.00 | 0.00 |
| ATOM | 170 | CA | THR | 2 | 278 | 23.206 | 72.798 | 53.406 | 1.00 | 0.00 |
| ATOM | 171 | C | THR | 2 | 278 | 22.141 | 71.927 | 52.704 | 1.00 | 0.00 |
| ATOM | 172 | O | THR | 2 | 278 | 21.101 | 72.343 | 52.185 | 1.00 | 0.00 |
| ATOM | 173 | CB | THR | 2 | 278 | 22.674 | 74.004 | 54.219 | 1.00 | 0.00 |
| ATOM | 174 | OG1 | THR | 2 | 278 | 21.861 | 73.627 | 55.344 | 1.00 | 0.00 |
| ATOM | 175 | CG2 | THR | 2 | 278 | 21.993 | 75.073 | 53.358 | 1.00 | 0.00 |
| ATOM | 176 | H | THR | 2 | 278 | 24.785 | 74.138 | 52.856 | 1.00 | 0.00 |
| ATOM | 177 | HG1 | THR | 2 | 278 | 22.073 | 74.231 | 56.053 | 1.00 | 0.00 |
| ATOM | 178 | N | GLU | 2 | 279 | 22.488 | 70.623 | 53.704 | 1.00 | 0.00 |
| ATOM | 179 | CA | GLU | 2 | 279 | 21.927 | 69.631 | 51.778 | 1.00 | 0.00 |
| ATOM | 180 | C | GLU | 2 | 279 | 21.921 | 70.050 | 50.316 | 1.00 | 0.00 |
| ATOM | 181 | O | GLU | 2 | 279 | 21.165 | 70.913 | 49.854 | 1.00 | 0.00 |
| ATOM | 182 | CB | GLU | 2 | 279 | 20.592 | 69.032 | 52.246 | 1.00 | 0.00 |
| ATOM | 183 | CG | GLU | 2 | 279 | 20.020 | 67.960 | 51.297 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 184 | CD | GLU | 2 | 279 | 19.094 | 68.609 | 50.283 | 1.00 | 0.00 |
| ATOM | 185 | OE1 | GLU | 2 | 279 | 17.986 | 68.942 | 50.650 | 1.00 | 0.00 |
| ATOM | 186 | OE2 | GLU | 2 | 279 | 19.453 | 68.826 | 49.136 | 1.00 | 0.00 |
| ATOM | 187 | H | GLU | 2 | 279 | 23.386 | 70.431 | 53.090 | 1.00 | 0.00 |
| ATOM | 188 | N | ILE | 2 | 280 | 22.841 | 69.363 | 49.644 | 1.00 | 0.00 |
| ATOM | 189 | CA | ILE | 2 | 280 | 23.110 | 69.499 | 48.222 | 1.00 | 0.00 |
| ATOM | 190 | C | ILE | 2 | 280 | 22.881 | 68.131 | 47.609 | 1.00 | 0.00 |
| ATOM | 191 | O | ILE | 2 | 280 | 23.606 | 67.168 | 47.852 | 1.00 | 0.00 |
| ATOM | 192 | CB | ILE | 2 | 280 | 24.552 | 70.013 | 48.043 | 1.00 | 0.00 |
| ATOM | 193 | CG1 | ILE | 2 | 280 | 25.030 | 70.009 | 46.592 | 1.00 | 0.00 |
| ATOM | 194 | CG2 | ILE | 2 | 280 | 25.547 | 69.269 | 48.951 | 1.00 | 0.00 |
| ATOM | 195 | CD1 | ILE | 2 | 280 | 26.420 | 70.634 | 46.463 | 1.00 | 0.00 |
| ATOM | 196 | H | ILE | 2 | 280 | 23.311 | 68.638 | 50.148 | 1.00 | 0.00 |
| ATOM | 197 | N | ALA | 2 | 281 | 21.785 | 68.037 | 46.859 | 1.00 | 0.00 |
| ATOM | 198 | CA | ALA | 2 | 281 | 21.440 | 66.669 | 46.493 | 1.00 | 0.00 |
| ATOM | 199 | C | ALA | 2 | 281 | 22.028 | 66.231 | 45.172 | 1.00 | 0.00 |
| ATOM | 200 | O | ALA | 2 | 281 | 21.326 | 66.073 | 44.167 | 1.00 | 0.00 |
| ATOM | 201 | CB | ALA | 2 | 281 | 19.928 | 66.465 | 46.493 | 1.00 | 0.00 |
| ATOM | 202 | H | ALA | 2 | 281 | 21.266 | 68.813 | 46.512 | 1.00 | 0.00 |
| ATOM | 203 | N | TYR | 2 | 282 | 23.364 | 66.058 | 45.210 | 1.00 | 0.00 |
| ATOM | 204 | CA | TYR | 2 | 282 | 23.982 | 65.503 | 44.012 | 1.00 | 0.00 |
| ATOM | 205 | C | TYR | 2 | 282 | 23.504 | 64.093 | 43.724 | 1.00 | 0.00 |
| ATOM | 206 | O | TYR | 2 | 282 | 22.951 | 63.394 | 44.575 | 1.00 | 0.00 |
| ATOM | 207 | CB | TYR | 2 | 282 | 25.515 | 65.707 | 44.029 | 1.00 | 0.00 |
| ATOM | 208 | CG | TYR | 2 | 282 | 26.364 | 64.515 | 44.435 | 1.00 | 0.00 |
| ATOM | 209 | CD1 | TYR | 2 | 282 | 26.981 | 63.765 | 43.414 | 1.00 | 0.00 |
| ATOM | 210 | CD2 | TYR | 2 | 282 | 26.562 | 64.209 | 45.798 | 1.00 | 0.00 |
| ATOM | 211 | CE1 | TYR | 2 | 282 | 27.851 | 62.717 | 43.759 | 1.00 | 0.00 |
| ATOM | 212 | CE2 | TYR | 2 | 282 | 27.441 | 63.165 | 46.144 | 1.00 | 0.00 |
| ATOM | 213 | CZ | TYR | 2 | 282 | 28.084 | 62.436 | 45.120 | 1.00 | 0.00 |
| ATOM | 214 | OH | TYR | 2 | 282 | 28.959 | 61.406 | 45.442 | 1.00 | 0.00 |
| ATOM | 215 | H | TYR | 2 | 282 | 23.773 | 66.009 | 46.120 | 1.00 | 0.00 |
| ATOM | 216 | HH | TYR | 2 | 282 | 29.388 | 61.649 | 46.270 | 1.00 | 0.00 |
| ATOM | 217 | N | GLY | 2 | 283 | 23.667 | 63.706 | 42.474 | 1.00 | 0.00 |
| ATOM | 218 | CA | GLY | 2 | 283 | 22.968 | 62.498 | 42.089 | 1.00 | 0.00 |
| ATOM | 219 | C | GLY | 2 | 283 | 23.562 | 62.006 | 40.818 | 1.00 | 0.00 |
| ATOM | 220 | O | GLY | 2 | 283 | 24.474 | 62.628 | 40.270 | 1.00 | 0.00 |
| ATOM | 221 | H | GLY | 2 | 283 | 24.147 | 64.280 | 41.815 | 1.00 | 0.00 |
| ATOM | 222 | N | THR | 2 | 284 | 23.015 | 60.879 | 40.380 | 1.00 | 0.00 |
| ATOM | 223 | CA | THR | 2 | 284 | 23.772 | 60.075 | 39.428 | 1.00 | 0.00 |
| ATOM | 224 | C | THR | 2 | 284 | 22.893 | 59.153 | 38.616 | 1.00 | 0.00 |
| ATOM | 225 | O | THR | 2 | 284 | 21.764 | 58.788 | 38.984 | 1.00 | 0.00 |
| ATOM | 226 | CB | THR | 2 | 284 | 24.852 | 59.288 | 40.200 | 1.00 | 0.00 |
| ATOM | 227 | OG1 | THR | 2 | 284 | 25.764 | 58.575 | 39.343 | 1.00 | 0.00 |
| ATOM | 228 | CG2 | THR | 2 | 284 | 24.250 | 58.343 | 41.251 | 1.00 | 0.00 |
| ATOM | 229 | H | THR | 2 | 284 | 22.167 | 60.561 | 50.802 | 1.00 | 0.00 |
| ATOM | 230 | HG1 | THR | 2 | 284 | 25.479 | 57.664 | 39.436 | 1.00 | 0.00 |
| ATOM | 231 | N | LEU | 2 | 285 | 23.500 | 58.725 | 37.486 | 1.00 | 0.00 |
| ATOM | 232 | CA | LEU | 2 | 285 | 22.981 | 57.583 | 36.732 | 1.00 | 0.00 |
| ATOM | 233 | C | LEU | 2 | 285 | 22.958 | 56.318 | 37.570 | 1.00 | 0.00 |
| ATOM | 234 | O | LEU | 2 | 285 | 23.981 | 55.684 | 37.816 | 1.00 | 0.00 |
| ATOM | 235 | CB | LEU | 2 | 285 | 23.753 | 57.355 | 35.416 | 1.00 | 0.00 |
| ATOM | 236 | CG | LEU | 2 | 285 | 25.273 | 57.109 | 35.479 | 1.00 | 0.00 |
| ATOM | 237 | CD1 | LEU | 2 | 285 | 25.726 | 56.206 | 34.332 | 1.00 | 0.00 |
| ATOM | 238 | CD2 | LEU | 2 | 285 | 26.110 | 58.390 | 35.534 | 1.00 | 0.00 |
| ATOM | 239 | H | LEU | 2 | 285 | 24.324 | 59.245 | 37.263 | 1.00 | 0.00 |
| ATOM | 240 | N | ASP | 2 | 286 | 21.747 | 56.017 | 38.047 | 1.00 | 0.00 |
| ATOM | 241 | CA | ASP | 2 | 286 | 21.498 | 54.892 | 39.940 | 1.00 | 0.00 |
| ATOM | 242 | C | ASP | 2 | 286 | 22.270 | 53.604 | 38.675 | 1.00 | 0.00 |
| ATOM | 243 | O | ASP | 2 | 286 | 22.712 | 52.962 | 39.626 | 1.00 | 0.00 |
| ATOM | 244 | CB | ASP | 2 | 286 | 19.987 | 54.611 | 39.002 | 1.00 | 0.00 |
| ATOM | 245 | CG | ASP | 2 | 286 | 19.212 | 55.566 | 39.912 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 246 | OD1 | ASP | 2 | 286 | 19.369 | 56.781 | 39.852 | 1.00 | 0.00 |
| ATOM | 247 | OD2 | ASP | 2 | 286 | 18.404 | 55.090 | 40.695 | 1.00 | 0.00 |
| ATOM | 248 | H | ASP | 2 | 286 | 20.999 | 56.664 | 37.947 | 1.00 | 0.00 |
| ATOM | 249 | N | SER | 2 | 287 | 22.380 | 53.245 | 37.377 | 1.00 | 0.00 |
| ATOM | 250 | CA | SER | 2 | 287 | 23.007 | 51.964 | 37.030 | 1.00 | 0.00 |
| ATOM | 251 | C | SER | 2 | 287 | 24.504 | 51.867 | 37.330 | 1.00 | 0.00 |
| ATOM | 252 | O | SER | 2 | 287 | 25.076 | 50.802 | 37.554 | 1.00 | 0.00 |
| ATOM | 253 | CB | SER | 2 | 287 | 22.802 | 51.615 | 35.536 | 1.00 | 0.00 |
| ATOM | 254 | OG | SER | 2 | 287 | 21.462 | 51.866 | 35.069 | 1.00 | 0.00 |
| ATOM | 255 | H | SER | 2 | 287 | 22.187 | 53.919 | 36.661 | 1.00 | 0.00 |
| ATOM | 256 | HG | SER | 2 | 287 | 20.999 | 52.147 | 35.855 | 1.00 | 0.00 |
| ATOM | 257 | N | GLY | 2 | 288 | 25.167 | 53.031 | 37.230 | 1.00 | 0.00 |
| ATOM | 258 | CA | GLY | 2 | 288 | 26.626 | 52.984 | 37.096 | 1.00 | 0.00 |
| ATOM | 259 | C | GLY | 2 | 288 | 27.377 | 52.478 | 38.312 | 1.00 | 0.00 |
| ATOM | 260 | O | GLY | 2 | 288 | 27.650 | 53.230 | 39.243 | 1.00 | 0.00 |
| ATOM | 261 | H | GLY | 2 | 288 | 24.628 | 53.877 | 37.232 | 1.00 | 0.00 |
| ATOM | 262 | N | SER | 2 | 289 | 27.719 | 51.171 | 38.290 | 1.00 | 0.00 |
| ATOM | 263 | CA | SER | 2 | 289 | 28.385 | 50.590 | 39.470 | 1.00 | 0.00 |
| ATOM | 264 | C | SER | 2 | 289 | 29.704 | 51.269 | 39.806 | 1.00 | 0.00 |
| ATOM | 265 | O | SER | 2 | 289 | 29.976 | 51.724 | 40.915 | 1.00 | 0.00 |
| ATOM | 266 | CB | SER | 2 | 289 | 28.590 | 49.078 | 39.285 | 1.00 | 0.00 |
| ATOM | 267 | OG | SER | 2 | 289 | 29.316 | 48.500 | 40.387 | 1.00 | 0.00 |
| ATOM | 268 | H | SER | 2 | 289 | 27.456 | 50.611 | 37.499 | 1.00 | 0.00 |
| ATOM | 269 | HG | SER | 2 | 289 | 28.731 | 48.548 | 41.142 | 1.00 | 0.00 |
| ATOM | 270 | N | THR | 2 | 290 | 30.526 | 51.368 | 38.759 | 1.00 | 0.00 |
| ATOM | 271 | CA | THR | 2 | 290 | 31.748 | 52.134 | 38.962 | 1.00 | 0.00 |
| ATOM | 272 | C | THR | 2 | 290 | 31.539 | 53.581 | 39.389 | 1.00 | 0.00 |
| ATOM | 273 | O | THR | 2 | 290 | 32.361 | 54.179 | 40.073 | 1.00 | 0.00 |
| ATOM | 274 | CB | THR | 2 | 290 | 32.627 | 52.021 | 37.719 | 1.00 | 0.00 |
| ATOM | 275 | OG1 | THR | 2 | 290 | 31.837 | 51.651 | 36.571 | 1.00 | 0.00 |
| ATOM | 276 | CG2 | THR | 2 | 290 | 33.738 | 50.994 | 37.944 | 1.00 | 0.00 |
| ATOM | 277 | H | THR | 2 | 290 | 30.222 | 51.165 | 37.830 | 1.00 | 0.00 |
| ATOM | 278 | HG1 | THR | 2 | 290 | 32.377 | 51.096 | 35.999 | 1.00 | 0.00 |
| ATOM | 279 | N | LYS | 2 | 2901 | 30.392 | 54.153 | 38.992 | 1.00 | 0.00 |
| ATOM | 280 | CA | LYS | 2 | 2901 | 30.094 | 55.503 | 39.487 | 1.00 | 0.00 |
| ATOM | 281 | C | LYS | 2 | 2901 | 29.635 | 55.560 | 40.940 | 1.00 | 0.00 |
| ATOM | 282 | O | LYS | 2 | 2901 | 29.947 | 56.483 | 41.678 | 1.00 | 0.00 |
| ATOM | 283 | CB | LYS | 2 | 2901 | 29.128 | 56.262 | 38.566 | 1.00 | 0.00 |
| ATOM | 284 | CG | LYS | 2 | 2901 | 29.702 | 56.615 | 37.185 | 1.00 | 0.00 |
| ATOM | 285 | CD | LYS | 2 | 2901 | 29.647 | 55.485 | 36.151 | 1.00 | 0.00 |
| ATOM | 286 | CE | LYS | 2 | 2901 | 30.302 | 55.839 | 34.814 | 1.00 | 0.00 |
| ATOM | 287 | NZ | LYS | 2 | 2901 | 31.765 | 55.879 | 34.951 | 1.00 | 0.00 |
| ATOM | 288 | H | LYS | 2 | 2901 | 29.714 | 53.581 | 38.523 | 1.00 | 0.00 |
| ATOM | 289 | 1HZ | LYS | 2 | 2901 | 32.233 | 56.069 | 34.047 | 1.00 | 0.00 |
| ATOM | 290 | 2HZ | LYS | 2 | 2901 | 32.081 | 56.627 | 35.591 | 1.00 | 0.00 |
| ATOM | 291 | 3HZ | LYS | 2 | 2901 | 32.185 | 55.008 | 35.303 | 1.00 | 0.00 |
| ATOM | 292 | N | GLU | 2 | 291 | 28.945 | 54.474 | 41.341 | 1.00 | 0.00 |
| ATOM | 293 | CA | GLU | 2 | 291 | 28.532 | 54.306 | 42.737 | 1.00 | 0.00 |
| ATOM | 294 | C | GLU | 2 | 291 | 29.727 | 54.367 | 43.675 | 1.00 | 0.00 |
| ATOM | 295 | O | GLU | 2 | 291 | 29.695 | 54.985 | 44.732 | 1.00 | 0.00 |
| ATOM | 296 | CB | GLU | 2 | 291 | 27.761 | 52.982 | 42.873 | 1.00 | 0.00 |
| ATOM | 297 | CG | GLU | 2 | 291 | 26.958 | 52.724 | 44.160 | 1.00 | 0.00 |
| ATOM | 298 | CD | GLU | 2 | 291 | 27.841 | 52.600 | 45.391 | 1.00 | 0.00 |
| ATOM | 299 | OE1 | GLU | 2 | 291 | 27.557 | 53.263 | 46.380 | 1.00 | 0.00 |
| ATOM | 300 | OE2 | GLU | 2 | 291 | 28.820 | 51.862 | 45.380 | 1.00 | 0.00 |
| ATOM | 301 | H | GLU | 2 | 291 | 28.838 | 53.748 | 40.663 | 1.00 | 0.00 |
| ATOM | 302 | N | PHE | 2 | 292 | 30.799 | 53.720 | 43.178 | 1.00 | 0.00 |
| ATOM | 303 | CA | PHE | 2 | 292 | 32.086 | 53.928 | 43.833 | 1.00 | 0.00 |
| ATOM | 304 | C | PHE | 2 | 292 | 32.600 | 55.351 | 43.688 | 1.00 | 0.00 |
| ATOM | 305 | O | PHE | 2 | 292 | 32.199 | 56.151 | 44.619 | 1.00 | 0.00 |
| ATOM | 306 | CB | PHE | 2 | 292 | 33.131 | 52.899 | 43.368 | 1.00 | 0.00 |
| ATOM | 307 | CG | PHE | 2 | 292 | 32.589 | 51.486 | 43.412 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 308 | CD1 | PHE | 2 | 292 | 32.575 | 50.730 | 42.221 | 1.00 | 0.00 |
| ATOM | 309 | CD2 | PHE | 2 | 292 | 32.109 | 50.943 | 44.625 | 1.00 | 0.00 |
| ATOM | 310 | CE1 | PHE | 2 | 292 | 32.055 | 49.422 | 42.233 | 1.00 | 0.00 |
| ATOM | 311 | CE2 | PHE | 2 | 292 | 31.587 | 49.635 | 44.641 | 1.00 | 0.00 |
| ATOM | 312 | CZ | PHE | 2 | 292 | 31.558 | 48.891 | 43.442 | 1.00 | 0.00 |
| ATOM | 313 | H | PHE | 2 | 292 | 60.681 | 53.226 | 42.313 | 1.00 | 0.00 |
| ATOM | 314 | N | PHE | 2 | 293 | 33.113 | 55.616 | 42.468 | 1.00 | 0.00 |
| ATOM | 315 | CA | PHE | 2 | 293 | 33.979 | 56.765 | 42.193 | 1.00 | 0.00 |
| ATOM | 316 | C | PHE | 2 | 293 | 33.633 | 58.054 | 42.925 | 1.00 | 0.00 |
| ATOM | 317 | O | PHE | 2 | 293 | 34.204 | 58.388 | 43.958 | 1.00 | 0.00 |
| ATOM | 318 | CB | PHE | 2 | 293 | 34.072 | 56.947 | 40.667 | 1.00 | 0.00 |
| ATOM | 319 | CG | PHE | 2 | 293 | 35.180 | 57.893 | 40.263 | 1.00 | 0.00 |
| ATOM | 320 | CD1 | PHE | 2 | 293 | 34.846 | 59.172 | 39.767 | 1.00 | 0.00 |
| ATOM | 321 | CD2 | PHE | 2 | 293 | 36.527 | 47.482 | 40.372 | 1.00 | 0.00 |
| ATOM | 322 | CE1 | PHE | 2 | 293 | 35.870 | 60.052 | 39.368 | 1.00 | 0.00 |
| ATOM | 323 | CE2 | PHE | 2 | 293 | 37.553 | 58.361 | 39.974 | 1.00 | 0.00 |
| ATOM | 324 | CZ | PHE | 2 | 293 | 37.214 | 59.636 | 39.472 | 1.00 | 0.00 |
| ATOM | 325 | H | PHE | 2 | 293 | 32.949 | 54.926 | 41.766 | 1.00 | 0.00 |
| ATOM | 326 | N | ARG | 2 | 294 | 32.632 | 58.759 | 42.373 | 1.00 | 0.00 |
| ATOM | 327 | CA | ARG | 2 | 294 | 32.265 | 60.046 | 42.969 | 1.00 | 0.00 |
| ATOM | 328 | C | ARG | 2 | 294 | 31.877 | 59.981 | 44.442 | 1.00 | 0.00 |
| ATOM | 329 | O | ARG | 2 | 294 | 32.233 | 60.840 | 45.248 | 1.00 | 0.00 |
| ATOM | 330 | CB | ARG | 2 | 294 | 31.185 | 60.741 | 42.129 | 1.00 | 0.00 |
| ATOM | 331 | CG | ARG | 2 | 294 | 31.156 | 62.270 | 42.283 | 1.00 | 0.00 |
| ATOM | 332 | CD | ARG | 2 | 294 | 32.400 | 62.957 | 41.708 | 1.00 | 0.00 |
| ATOM | 333 | NE | ARG | 2 | 294 | 32.390 | 64.400 | 41.952 | 1.00 | 0.00 |
| ATOM | 334 | CZ | ARG | 2 | 294 | 33.419 | 65.174 | 41.524 | 1.00 | 0.00 |
| ATOM | 335 | NH1 | ARG | 2 | 294 | 33.445 | 66.439 | 41.891 | 1.00 | 0.00 |
| ATOM | 336 | NH2 | ARG | 2 | 294 | 34.400 | 64.693 | 40.757 | 1.00 | 0.00 |
| ATOM | 337 | H | ARG | 2 | 294 | 32.123 | 58.395 | 41.600 | 1.00 | 0.00 |
| ATOM | 338 | HE | ARG | 2 | 294 | 31.655 | 64.819 | 42.507 | 1.00 | 0.00 |
| ATOM | 339 | 1HH1 | ARG | 2 | 294 | 34.186 | 67.045 | 41.616 | 1.00 | 0.00 |
| ATOM | 340 | 2HH1 | ARG | 2 | 294 | 32.712 | 66.787 | 42.483 | 1.00 | 0.00 |
| ATOM | 341 | 1HH2 | ARG | 2 | 294 | 34.323 | 63.790 | 40.345 | 1.00 | 0.00 |
| ATOM | 342 | 2HH2 | ARG | 2 | 294 | 35.215 | 65.268 | 40.614 | 1.00 | 0.00 |
| ATOM | 343 | N | ARG | 2 | 295 | 31.175 | 58.888 | 44.788 | 1.00 | 0.00 |
| ATOM | 344 | CA | ARG | 2 | 295 | 30.829 | 58.695 | 46.200 | 1.00 | 0.00 |
| ATOM | 345 | C | ARG | 2 | 295 | 31.999 | 58.531 | 47.171 | 1.00 | 0.00 |
| ATOM | 346 | O | ARG | 2 | 295 | 31.906 | 58.823 | 48.365 | 1.00 | 0.00 |
| ATOM | 347 | CB | ARG | 2 | 295 | 29.797 | 57.566 | 46.302 | 1.00 | 0.00 |
| ATOM | 348 | CG | ARG | 2 | 295 | 29.245 | 57.202 | 47.687 | 1.00 | 0.00 |
| ATOM | 349 | CD | ARG | 2 | 295 | 30.019 | 56.113 | 48.436 | 1.00 | 0.00 |
| ATOM | 350 | NE | ARG | 2 | 295 | 29.886 | 54.810 | 47.786 | 1.00 | 0.00 |
| ATOM | 351 | CZ | ARG | 2 | 295 | 30.945 | 54.128 | 47.324 | 1.00 | 0.00 |
| ATOM | 352 | NH1 | ARG | 2 | 295 | 30.742 | 52.903 | 46.878 | 1.00 | 0.00 |
| ATOM | 353 | NH2 | ARG | 2 | 295 | 32.161 | 54.668 | 47.312 | 1.00 | 0.00 |
| ATOM | 354 | H | ARG | 2 | 295 | 30.931 | 58.229 | 44.077 | 1.00 | 0.00 |
| ATOM | 355 | HE | ARG | 2 | 295 | 29.003 | 54.347 | 47.661 | 1.00 | 0.00 |
| ATOM | 356 | 1HH1 | ARG | 2 | 295 | 31.467 | 52.248 | 46.680 | 1.00 | 0.00 |
| ATOM | 357 | 2HH1 | ARG | 2 | 295 | 29.786 | 52.606 | 46.720 | 1.00 | 0.00 |
| ATOM | 358 | 1HH2 | ARG | 2 | 295 | 32.948 | 54.187 | 46.928 | 1.00 | 0.00 |
| ATOM | 359 | 2HH2 | ARG | 2 | 295 | 32.310 | 55.591 | 47.668 | 1.00 | 0.00 |
| ATOM | 360 | N | SER | 2 | 296 | 33.131 | 58.065 | 46.626 | 1.00 | 0.00 |
| ATOM | 361 | CA | SER | 2 | 296 | 34.260 | 57.764 | 47.512 | 1.00 | 0.00 |
| ATOM | 362 | C | SER | 2 | 296 | 34.869 | 58.924 | 48.300 | 1.00 | 0.00 |
| ATOM | 363 | O | SER | 2 | 296 | 35.612 | 58.735 | 49.261 | 1.00 | 0.00 |
| ATOM | 364 | CB | SER | 2 | 296 | 35.296 | 56.934 | 46.754 | 1.00 | 0.00 |
| ATOM | 365 | OG | SER | 2 | 296 | 34.608 | 55.845 | 46.096 | 1.00 | 0.00 |
| ATOM | 366 | H | SER | 2 | 296 | 33.146 | 57.881 | 45.643 | 1.00 | 0.00 |
| ATOM | 367 | HG | SER | 2 | 296 | 34.395 | 56.177 | 45.217 | 1.00 | 0.00 |
| ATOM | 368 | N | LYS | 2 | 297 | 34.438 | 60.139 | 47.916 | 1.00 | 0.00 |
| ATOM | 369 | CA | LYS | 2 | 297 | 34.660 | 61.363 | 48.681 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 370 | C | LYS | 2 | 297 | 34.436 | 61.225 | 50.186 | 1.00 | 0.00 |
| ATOM | 371 | O | LYS | 2 | 297 | 35.230 | 61.701 | 50.983 | 1.00 | 0.00 |
| ATOM | 372 | CB | LYS | 2 | 297 | 33.829 | 52.471 | 48.020 | 1.00 | 0.00 |
| ATOM | 373 | CG | LYS | 2 | 297 | 34.223 | 63.921 | 48.318 | 1.00 | 0.00 |
| ATOM | 374 | CD | LYS | 2 | 297 | 33.804 | 64.829 | 47.153 | 1.00 | 0.00 |
| ATOM | 375 | CE | LYS | 2 | 297 | 34.072 | 66.324 | 47.361 | 1.00 | 0.00 |
| ATOM | 376 | NZ | LYS | 2 | 297 | 33.055 | 66.888 | 48.250 | 1.00 | 0.00 |
| ATOM | 377 | H | LYS | 2 | 297 | 33.888 | 60.186 | 47.087 | 1.00 | 0.00 |
| ATOM | 378 | 1HZ | LYS | 2 | 297 | 32.862 | 66.272 | 49.065 | 1.00 | 0.00 |
| ATOM | 379 | 2HZ | LYS | 2 | 297 | 33.404 | 67.770 | 48.686 | 1.00 | 0.00 |
| ATOM | 380 | 3HZ | LYS | 2 | 297 | 32.157 | 67.089 | 47.767 | 1.00 | 0.00 |
| ATOM | 381 | N | ILE | 2 | 298 | 33.384 | 60.468 | 50.539 | 1.00 | 0.00 |
| ATOM | 382 | CA | ILE | 2 | 298 | 33.172 | 60.218 | 41.981 | 1.00 | 0.00 |
| ATOM | 383 | C | ILE | 2 | 298 | 34.255 | 59.388 | 52.672 | 1.00 | 0.00 |
| ATOM | 384 | O | ILE | 2 | 298 | 34.600 | 59.592 | 53.830 | 1.00 | 0.00 |
| ATOM | 385 | CB | ILE | 2 | 298 | 31.750 | 59.669 | 52.209 | 1.00 | 0.00 |
| ATOM | 386 | CG1 | ILE | 2 | 298 | 31.360 | 59.681 | 53.689 | 1.00 | 0.00 |
| ATOM | 387 | CG2 | ILE | 2 | 298 | 31.568 | 58.269 | 51.603 | 1.00 | 0.00 |
| ATOM | 388 | CD1 | ILE | 2 | 298 | 29.886 | 59.336 | 53.917 | 1.00 | 0.00 |
| ATOM | 389 | H | ILE | 2 | 298 | 32.831 | 60.019 | 49.838 | 1.00 | 0.00 |
| ATOM | 390 | N | ALA | 2 | 299 | 34.810 | 58.432 | 51.907 | 1.00 | 0.00 |
| ATOM | 391 | CA | ALA | 2 | 299 | 35.835 | 57.551 | 52.474 | 1.00 | 0.00 |
| ATOM | 392 | C | ALA | 2 | 299 | 37.203 | 58.198 | 52.590 | 1.00 | 0.00 |
| ATOM | 393 | O | ALA | 2 | 299 | 37.986 | 57.932 | 53.496 | 1.00 | 0.00 |
| ATOM | 394 | CB | ALA | 2 | 299 | 35.957 | 56.272 | 51.644 | 1.00 | 0.00 |
| ATOM | 395 | H | ALA | 2 | 299 | 34.555 | 58.334 | 50.947 | 1.00 | 0.00 |
| ATOM | 396 | N | VAL | 2 | 300 | 37.449 | 59.113 | 51.643 | 1.00 | 0.00 |
| ATOM | 397 | CA | VAL | 2 | 300 | 38.522 | 60.069 | 51.905 | 1.00 | 0.00 |
| ATOM | 398 | C | VAL | 2 | 300 | 37.920 | 61.305 | 52.554 | 1.00 | 0.00 |
| ATOM | 399 | O | VAL | 2 | 300 | 37.738 | 52.337 | 51.918 | 1.00 | 0.00 |
| ATOM | 400 | CB | VAL | 2 | 300 | 39.273 | 60.411 | 50.608 | 1.00 | 0.00 |
| ATOM | 401 | CG1 | VAL | 2 | 300 | 40.550 | 61.211 | 50.893 | 1.00 | 0.00 |
| ATOM | 402 | CG2 | VAL | 2 | 300 | 39.583 | 59.151 | 49.794 | 1.00 | 0.00 |
| ATOM | 403 | H | VAL | 2 | 300 | 36.828 | 59.223 | 50.868 | 1.00 | 0.00 |
| ATOM | 404 | N | TYR | 2 | 301 | 37.542 | 61.087 | 53.825 | 1.00 | 0.00 |
| ATOM | 405 | CA | TYR | 2 | 301 | 36.597 | 61.901 | 54.603 | 1.00 | 0.00 |
| ATOM | 406 | C | TYR | 2 | 301 | 36.372 | 63.395 | 54.374 | 1.00 | 0.00 |
| ATOM | 407 | O | TYR | 2 | 301 | 36.581 | 64.209 | 55.275 | 1.00 | 0.00 |
| ATOM | 408 | CB | TYR | 2 | 301 | 36.816 | 61.647 | 56.101 | 1.00 | 0.00 |
| ATOM | 409 | CG | TYR | 2 | 301 | 36.279 | 60.295 | 56.519 | 1.00 | 0.00 |
| ATOM | 410 | CD1 | TYR | 2 | 301 | 37.163 | 59.202 | 56.629 | 1.00 | 0.00 |
| ATOM | 411 | CD2 | TYR | 2 | 301 | 34.903 | 60.170 | 56.804 | 1.00 | 0.00 |
| ATOM | 412 | CE1 | TYR | 2 | 301 | 36.663 | 57.959 | 57.056 | 1.00 | 0.00 |
| ATOM | 413 | CE2 | TYR | 2 | 301 | 34.402 | 58.926 | 57.222 | 1.00 | 0.00 |
| ATOM | 414 | CZ | TYR | 2 | 301 | 35.290 | 57.840 | 57.356 | 1.00 | 0.00 |
| ATOM | 415 | OH | TYR | 2 | 301 | 34.795 | 56.627 | 57.804 | 1.00 | 0.00 |
| ATOM | 416 | H | TYR | 2 | 301 | 37.815 | 60.200 | 54.197 | 1.00 | 0.00 |
| ATOM | 417 | HH | TYR | 2 | 301 | 35.421 | 56.250 | 58.417 | 1.00 | 0.00 |
| ATOM | 418 | N | GLU | 2 | 302 | 35.833 | 63.716 | 53.190 | 1.00 | 0.00 |
| ATOM | 419 | CA | GLU | 2 | 302 | 34.943 | 64.873 | 53.164 | 1.00 | 0.00 |
| ATOM | 420 | C | GLU | 2 | 302 | 33.539 | 64.323 | 53.615 | 1.00 | 0.00 |
| ATOM | 421 | O | GLU | 2 | 302 | 33.289 | 63.170 | 52.963 | 1.00 | 0.00 |
| ATOM | 422 | CB | GLU | 2 | 302 | 35.149 | 65.690 | 51.879 | 1.00 | 0.00 |
| ATOM | 423 | CG | GLU | 2 | 302 | 34.482 | 67.078 | 51.885 | 1.00 | 0.00 |
| ATOM | 424 | CD | GLU | 2 | 302 | 33.216 | 67.115 | 51.041 | 1.00 | 0.00 |
| ATOM | 425 | OE1 | GLU | 2 | 302 | 32.860 | 68.171 | 50.540 | 1.00 | 0.00 |
| ATOM | 426 | OE2 | GLU | 2 | 302 | 32.581 | 66.097 | 50.813 | 1.00 | 0.00 |
| ATOM | 427 | H | GLU | 2 | 302 | 35.880 | 63.072 | 52.426 | 1.00 | 0.00 |
| ATOM | 428 | N | LYS | 2 | 303 | 32.647 | 65.135 | 53.908 | 1.00 | 0.00 |
| ATOM | 429 | CA | LYS | 2 | 303 | 31.351 | 64.595 | 54.322 | 1.00 | 0.00 |
| ATOM | 430 | C | LYS | 2 | 303 | 30.584 | 63.858 | 53.232 | 1.00 | 0.00 |
| ATOM | 431 | O | LYS | 2 | 303 | 30.059 | 62.767 | 53.437 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 432 | CB | LYS | 2 | 303 | 30.512 | 65.703 | 54.978 | 1.00 | 0.00 |
| ATOM | 433 | CG | LYS | 2 | 303 | 29.155 | 65.246 | 55.533 | 1.00 | 0.00 |
| ATOM | 434 | CD | LYS | 2 | 303 | 27.983 | 65.801 | 54.720 | 1.00 | 0.00 |
| ATOM | 435 | CE | LYS | 2 | 303 | 27.837 | 67.309 | 54.903 | 1.00 | 0.00 |
| ATOM | 436 | NZ | LYS | 2 | 303 | 27.006 | 67.885 | 53.840 | 1.00 | 0.00 |
| ATOM | 437 | H | LYS | 2 | 303 | 32.971 | 66.061 | 54.092 | 1.00 | 0.00 |
| ATOM | 438 | 1HZ | LYS | 2 | 303 | 27.406 | 67.678 | 52.903 | 1.00 | 0.00 |
| ATOM | 439 | 2HZ | LYS | 2 | 303 | 26.054 | 67.481 | 53.894 | 1.00 | 0.00 |
| ATOM | 440 | 3HZ | LYS | 2 | 303 | 26.993 | 68.921 | 53.937 | 1.00 | 0.00 |
| ATOM | 441 | N | MET | 2 | 304 | 30.558 | 64.512 | 52.063 | 1.00 | 0.00 |
| ATOM | 442 | CA | MET | 2 | 304 | 29.870 | 64.040 | 50.859 | 1.00 | 0.00 |
| ATOM | 443 | C | MET | 2 | 304 | 28.349 | 64.030 | 50.863 | 1.00 | 0.00 |
| ATOM | 444 | O | MET | 2 | 304 | 27.735 | 64.443 | 49.879 | 1.00 | 0.00 |
| ATOM | 445 | CB | MET | 2 | 304 | 30.398 | 62.694 | 50.358 | 1.00 | 0.00 |
| ATOM | 446 | CG | MET | 2 | 304 | 29.915 | 62.406 | 48.938 | 1.00 | 0.00 |
| ATOM | 447 | SD | MET | 2 | 304 | 29.810 | 60.658 | 48.586 | 1.00 | 0.00 |
| ATOM | 448 | CE | MET | 2 | 304 | 28.597 | 60.203 | 49.831 | 1.00 | 0.00 |
| ATOM | 449 | H | MET | 2 | 304 | 31.067 | 65.371 | 51.993 | 1.00 | 0.00 |
| ATOM | 450 | N | TRP | 2 | 305 | 27.790 | 63.526 | 51.982 | 1.00 | 0.00 |
| ATOM | 451 | CA | TRP | 2 | 305 | 26.370 | 63.230 | 52.140 | 1.00 | 0.00 |
| ATOM | 452 | C | TRP | 2 | 305 | 25.942 | 62.087 | 51.242 | 1.00 | 0.00 |
| ATOM | 453 | O | TRP | 2 | 305 | 26.016 | 62.164 | 50.017 | 1.00 | 0.00 |
| ATOM | 454 | CB | TRP | 2 | 305 | 25.508 | 64.496 | 51.966 | 1.00 | 0.00 |
| ATOM | 455 | CG | TRP | 2 | 305 | 24.065 | 64.246 | 52.338 | 1.00 | 0.00 |
| ATOM | 456 | CD1 | TRP | 2 | 305 | 23.567 | 63.888 | 53.601 | 1.00 | 0.00 |
| ATOM | 457 | CD2 | TRP | 2 | 305 | 22.909 | 64.320 | 51.477 | 1.00 | 0.00 |
| ATOM | 458 | NE1 | TRP | 2 | 305 | 22.215 | 63.740 | 53.575 | 1.00 | 0.00 |
| ATOM | 459 | CE2 | TRP | 2 | 305 | 21.764 | 63.996 | 52.281 | 1.00 | 0.00 |
| ATOM | 460 | CE3 | TRP | 2 | 305 | 22.749 | 64.627 | 50.109 | 1.00 | 0.00 |
| ATOM | 461 | CZ2 | TRP | 2 | 305 | 20.480 | 63.984 | 51.695 | 1.00 | 0.00 |
| ATOM | 462 | CZ3 | TRP | 2 | 305 | 21.460 | 64.611 | 49.538 | 1.00 | 0.00 |
| ATOM | 463 | CH2 | TRP | 2 | 305 | 20.332 | 64.291 | 50.325 | 1.00 | 0.00 |
| ATOM | 464 | H | TRP | 2 | 305 | 28.425 | 63.168 | 52.656 | 1.00 | 0.00 |
| ATOM | 465 | HE1 | TRP | 2 | 305 | 21.643 | 63.522 | 54.345 | 1.00 | 0.00 |
| ATOM | 466 | N | SER | 2 | 306 | 25.472 | 61.008 | 51.890 | 1.00 | 0.00 |
| ATOM | 467 | CA | SER | 2 | 306 | 24.819 | 60.017 | 51.040 | 1.00 | 0.00 |
| ATOM | 468 | C | SER | 2 | 306 | 23.575 | 60.587 | 50.418 | 1.00 | 0.00 |
| ATOM | 469 | O | SER | 2 | 306 | 22.826 | 61.335 | 51.038 | 1.00 | 0.00 |
| ATOM | 470 | CB | SER | 2 | 306 | 24.564 | 58.715 | 51.778 | 1.00 | 0.00 |
| ATOM | 471 | OG | SER | 2 | 306 | 25.848 | 58.179 | 52.135 | 1.00 | 0.00 |
| ATOM | 472 | H | SER | 2 | 306 | 25.352 | 61.048 | 52.876 | 1.00 | 0.00 |
| ATOM | 473 | HG | SER | 2 | 306 | 26.425 | 58.942 | 52.074 | 1.00 | 0.00 |
| ATOM | 474 | N | TYR | 2 | 307 | 53.542 | 60.305 | 49.131 | 1.00 | 0.00 |
| ATOM | 475 | CA | TYR | 2 | 307 | 22.789 | 61.041 | 48.132 | 1.00 | 0.00 |
| ATOM | 476 | C | TYR | 2 | 307 | 22.098 | 59.957 | 47.345 | 1.00 | 0.00 |
| ATOM | 477 | O | TYR | 2 | 307 | 22.122 | 58.802 | 47.777 | 1.00 | 0.00 |
| ATOM | 478 | CB | TYR | 2 | 307 | 23.788 | 61.856 | 47.276 | 1.00 | 0.00 |
| ATOM | 479 | CG | TYR | 2 | 307 | 24.746 | 60.990 | 46.461 | 1.00 | 0.00 |
| ATOM | 480 | CD1 | TYR | 2 | 307 | 24.655 | 61.027 | 45.054 | 1.00 | 0.00 |
| ATOM | 481 | CD2 | TYR | 2 | 307 | 25.696 | 60.168 | 47.106 | 1.00 | 0.00 |
| ATOM | 482 | CE1 | TYR | 2 | 307 | 25.494 | 60.209 | 44.279 | 1.00 | 0.00 |
| ATOM | 483 | CE2 | TYR | 2 | 307 | 26.524 | 59.336 | 46.337 | 1.00 | 0.00 |
| ATOM | 484 | CZ | TYR | 2 | 307 | 26.409 | 59.361 | 44.934 | 1.00 | 0.00 |
| ATOM | 485 | OH | TYR | 2 | 307 | 27.227 | 58.533 | 44.186 | 1.00 | 0.00 |
| ATOM | 486 | H | TYR | 2 | 307 | 24.058 | 59.508 | 48.821 | 1.00 | 0.00 |
| ATOM | 487 | HH | TYR | 2 | 307 | 27.719 | 59.115 | 43.610 | 1.00 | 0.00 |
| ATOM | 488 | N | MET | 2 | 308 | 21.585 | 60.316 | 46.157 | 1.00 | 0.00 |
| ATOM | 489 | CA | MET | 2 | 308 | 21.196 | 59.236 | 45.255 | 1.00 | 0.00 |
| ATOM | 490 | C | MET | 2 | 308 | 22.196 | 58.087 | 45.149 | 1.00 | 0.00 |
| ATOM | 491 | O | MET | 2 | 308 | 23.422 | 58.226 | 45.165 | 1.00 | 0.00 |
| ATOM | 492 | CB | MET | 2 | 308 | 20.866 | 59.783 | 43.865 | 1.00 | 0.00 |
| ATOM | 493 | CG | MET | 2 | 308 | 19.888 | 60.959 | 43.910 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 494 | SD | MET | 2 | 308 | 19.528 | 61.631 | 42.281 | 1.00 | 0.00 |
| ATOM | 495 | CE | MET | 2 | 308 | 19.121 | 63.307 | 42.802 | 1.00 | 0.00 |
| ATOM | 496 | H | MET | 2 | 308 | 21.555 | 61.275 | 45.891 | 1.00 | 0.00 |
| ATOM | 497 | N | LYS | 2 | 309 | 21.585 | 56.898 | 45.081 | 1.00 | 0.00 |
| ATOM | 498 | CA | LYS | 2 | 309 | 22.342 | 55.679 | 44.798 | 1.00 | 0.00 |
| ATOM | 499 | C | LYS | 2 | 309 | 21.698 | 55.052 | 43.580 | 1.00 | 0.00 |
| ATOM | 500 | O | LYS | 2 | 309 | 21.109 | 55.783 | 42.791 | 1.00 | 0.00 |
| ATOM | 501 | CB | LYS | 2 | 309 | 22.337 | 54.753 | 46.021 | 1.00 | 0.00 |
| ATOM | 502 | CG | LYS | 2 | 309 | 23.731 | 54.603 | 46.638 | 1.00 | 0.00 |
| ATOM | 503 | CD | LYS | 2 | 309 | 24.264 | 55.907 | 47.236 | 1.00 | 0.00 |
| ATOM | 504 | CE | LYS | 2 | 309 | 25.748 | 55.854 | 47.593 | 1.00 | 0.00 |
| ATOM | 505 | NZ | LYS | 2 | 309 | 26.535 | 55.603 | 46.378 | 1.00 | 0.00 |
| ATOM | 506 | H | LYS | 2 | 309 | 20.584 | 56.895 | 45.110 | 1.00 | 0.00 |
| ATOM | 507 | 1HZ | LYS | 2 | 309 | 26.413 | 54.614 | 46.083 | 1.00 | 0.00 |
| ATOM | 508 | 2HZ | LYS | 2 | 309 | 26.265 | 56.222 | 45.592 | 1.00 | 0.00 |
| ATOM | 509 | 3HZ | LYS | 2 | 309 | 27.549 | 55.688 | 46.574 | 1.00 | 0.00 |
| ATOM | 510 | N | SER | 2 | 310 | 21.755 | 53.718 | 43.462 | 1.00 | 0.00 |
| ATOM | 511 | CA | SER | 2 | 310 | 20.764 | 53.046 | 42.617 | 1.00 | 0.00 |
| ATOM | 512 | C | SER | 2 | 310 | 19.398 | 52.988 | 43.305 | 1.00 | 0.00 |
| ATOM | 513 | O | SER | 2 | 310 | 18.987 | 51.965 | 43.839 | 1.00 | 0.00 |
| ATOM | 514 | CB | SER | 2 | 310 | 21.264 | 51.633 | 42.285 | 1.00 | 0.00 |
| ATOM | 515 | OG | SER | 2 | 310 | 22.661 | 51.655 | 41.940 | 1.00 | 0.00 |
| ATOM | 516 | H | SER | 2 | 310 | 22.365 | 53.129 | 43.995 | 1.00 | 0.00 |
| ATOM | 517 | HG | SER | 2 | 310 | 22.690 | 51.707 | 40.984 | 1.00 | 0.00 |
| ATOM | 518 | N | ALA | 2 | 311 | 18.737 | 54.155 | 43.323 | 1.00 | 0.00 |
| ATOM | 519 | CA | ALA | 2 | 311 | 17.644 | 54.346 | 44.279 | 1.00 | 0.00 |
| ATOM | 520 | C | ALA | 2 | 311 | 16.231 | 53.945 | 43.857 | 1.00 | 0.00 |
| ATOM | 521 | O | ALA | 2 | 311 | 15.469 | 53.382 | 44.641 | 1.00 | 0.00 |
| ATOM | 522 | CB | ALA | 2 | 311 | 17.649 | 55.790 | 44.785 | 1.00 | 0.00 |
| ATOM | 523 | H | ALA | 2 | 311 | 19.004 | 54.840 | 42.643 | 1.00 | 0.00 |
| ATOM | 524 | N | GLU | 2 | 312 | 15.884 | 54.240 | 42.597 | 1.00 | 0.00 |
| ATOM | 525 | CA | GLU | 2 | 312 | 14.538 | 53.848 | 42.191 | 1.00 | 0.00 |
| ATOM | 526 | C | GLU | 2 | 312 | 14.656 | 52.729 | 41.172 | 1.00 | 0.00 |
| ATOM | 527 | O | GLU | 2 | 312 | 15.185 | 52.945 | 40.087 | 1.00 | 0.00 |
| ATOM | 528 | CB | GLU | 2 | 312 | 13.749 | 55.044 | 41.617 | 1.00 | 0.00 |
| ATOM | 529 | CG | GLU | 2 | 312 | 12.956 | 55.912 | 42.620 | 1.00 | 0.00 |
| ATOM | 530 | CD | GLU | 2 | 312 | 13.716 | 57.137 | 43.124 | 1.00 | 0.00 |
| ATOM | 531 | OE1 | GLU | 2 | 312 | 14.834 | 56.999 | 43.604 | 1.00 | 0.00 |
| ATOM | 532 | OE2 | GLU | 2 | 312 | 13.190 | 58.250 | 43.048 | 1.00 | 0.00 |
| ATOM | 533 | H | GLU | 2 | 312 | 16.556 | 54.565 | 41.932 | 1.00 | 0.00 |
| ATOM | 534 | N | PRO | 2 | 313 | 14.190 | 51.520 | 41.549 | 1.00 | 0.00 |
| ATOM | 535 | CA | PRO | 2 | 313 | 14.325 | 50.369 | 40.646 | 1.00 | 0.00 |
| ATOM | 536 | C | PRO | 2 | 313 | 13.242 | 50.430 | 39.568 | 1.00 | 0.00 |
| ATOM | 537 | O | PRO | 2 | 313 | 12.575 | 49.318 | 39.349 | 1.00 | 0.00 |
| ATOM | 538 | CB | PRO | 2 | 313 | 14.243 | 49.207 | 41.640 | 1.00 | 0.00 |
| ATOM | 539 | CG | PRO | 2 | 313 | 13.275 | 49.692 | 42.721 | 1.00 | 0.00 |
| ATOM | 540 | CD | PRO | 2 | 313 | 13.613 | 51.173 | 42.844 | 1.00 | 0.00 |
| ATOM | 541 | N | SER | 2 | 314 | 13.061 | 51.461 | 38.909 | 1.00 | 0.00 |
| ATOM | 542 | CA | SER | 2 | 314 | 11.891 | 51.632 | 38.056 | 1.00 | 0.00 |
| ATOM | 543 | C | SER | 2 | 314 | 12.052 | 51.203 | 36.606 | 1.00 | 0.00 |
| ATOM | 544 | O | SER | 2 | 314 | 11.918 | 52.010 | 35.687 | 1.00 | 0.00 |
| ATOM | 545 | CB | SER | 2 | 314 | 11.434 | 53.084 | 38.174 | 1.00 | 0.00 |
| ATOM | 546 | OG | SER | 2 | 314 | 12.532 | 53.858 | 38.679 | 1.00 | 0.00 |
| ATOM | 547 | H | SER | 2 | 314 | 13.682 | 52.232 | 39.045 | 1.00 | 0.00 |
| ATOM | 548 | HG | SER | 2 | 314 | 12.494 | 54.717 | 38.259 | 1.00 | 0.00 |
| ATOM | 549 | N | VAL | 2 | 315 | 12.290 | 49.887 | 36.485 | 1.00 | 0.00 |
| ATOM | 550 | CA | VAL | 2 | 315 | 12.253 | 49.121 | 35.237 | 1.00 | 0.00 |
| ATOM | 551 | C | VAL | 2 | 315 | 13.345 | 49.363 | 34.197 | 1.00 | 0.00 |
| ATOM | 552 | O | VAL | 2 | 315 | 13.970 | 48.426 | 33.709 | 1.00 | 0.00 |
| ATOM | 553 | CB | VAL | 2 | 315 | 10.843 | 49.138 | 34.602 | 1.00 | 0.00 |
| ATOM | 554 | CG1 | VAL | 2 | 315 | 10.717 | 48.145 | 33.442 | 1.00 | 0.00 |
| ATOM | 555 | CG2 | VAL | 2 | 315 | 9.757 | 48.853 | 35.645 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 556 | H | VAL | 2 | 315 | 12.470 | 49.399 | 37.341 | 1.00 | 0.00 |
| ATOM | 557 | N | PHE | 2 | 316 | 13.502 | 50.623 | 33.799 | 1.00 | 0.00 |
| ATOM | 558 | CA | PHE | 2 | 316 | 14.526 | 50.909 | 32.800 | 1.00 | 0.00 |
| ATOM | 559 | C | PHE | 2 | 316 | 15.444 | 51.993 | 33.297 | 1.00 | 0.00 |
| ATOM | 560 | O | PHE | 2 | 316 | 15.137 | 52.718 | 34.246 | 1.00 | 0.00 |
| ATOM | 561 | CB | PHE | 2 | 316 | 13.907 | 51.367 | 31.473 | 1.00 | 0.00 |
| ATOM | 562 | CG | PHE | 2 | 316 | 13.084 | 50.279 | 30.822 | 1.00 | 0.00 |
| ATOM | 563 | CD1 | PHE | 2 | 316 | 11.706 | 50.500 | 30.611 | 1.00 | 0.00 |
| ATOM | 564 | CD2 | PHE | 2 | 316 | 13.699 | 49.071 | 30.423 | 1.00 | 0.00 |
| ATOM | 565 | CE1 | PHE | 2 | 316 | 10.931 | 49.503 | 29.987 | 1.00 | 0.00 |
| ATOM | 566 | CE2 | PHE | 2 | 316 | 12.926 | 48.072 | 29.802 | 1.00 | 0.00 |
| ATOM | 567 | CZ | PHE | 2 | 316 | 11.549 | 48.299 | 29.589 | 1.00 | 0.00 |
| ATOM | 568 | H | PHE | 2 | 316 | 13.059 | 51.354 | 34.314 | 1.00 | 0.00 |
| ATOM | 569 | N | THR | 2 | 317 | 16.572 | 52.155 | 32.580 | 1.00 | 0.00 |
| ATOM | 570 | CA | THR | 2 | 317 | 17.449 | 53.238 | 33.035 | 1.00 | 0.00 |
| ATOM | 571 | C | THR | 2 | 317 | 16.789 | 54.623 | 33.035 | 1.00 | 0.00 |
| ATOM | 572 | O | THR | 2 | 317 | 16.737 | 55.301 | 34.061 | 1.00 | 0.00 |
| ATOM | 573 | CB | THR | 2 | 317 | 18.840 | 53.169 | 32.367 | 1.00 | 0.00 |
| ATOM | 574 | OG1 | THR | 2 | 317 | 19.778 | 54.041 | 33.020 | 1.00 | 0.00 |
| ATOM | 575 | CG2 | THR | 2 | 317 | 18.827 | 53.399 | 30.852 | 1.00 | 0.00 |
| ATOM | 576 | H | THR | 2 | 317 | 16.855 | 51.477 | 31.903 | 1.00 | 0.00 |
| ATOM | 577 | HG1 | THR | 2 | 317 | 19.699 | 53.845 | 33.959 | 1.00 | 0.00 |
| ATOM | 578 | N | LYS | 2 | 318 | 16.149 | 54.962 | 31.888 | 1.00 | 0.00 |
| ATOM | 579 | CA | LYS | 2 | 318 | 15.389 | 56.221 | 31.815 | 1.00 | 0.00 |
| ATOM | 580 | C | LYS | 2 | 318 | 14.522 | 56.613 | 33.016 | 1.00 | 0.00 |
| ATOM | 581 | O | LYS | 2 | 318 | 14.302 | 57.799 | 33.283 | 1.00 | 0.00 |
| ATOM | 582 | CB | LYS | 2 | 318 | 14.572 | 56.276 | 30.506 | 1.00 | 0.00 |
| ATOM | 583 | CG | LYS | 2 | 318 | 13.743 | 57.557 | 30.288 | 1.00 | 0.00 |
| ATOM | 584 | CD | LYS | 2 | 318 | 12.238 | 57.373 | 30.548 | 1.00 | 0.00 |
| ATOM | 585 | CE | LYS | 2 | 318 | 11.545 | 58.533 | 31.285 | 1.00 | 0.00 |
| ATOM | 586 | NZ | LYS | 2 | 318 | 11.767 | 58.443 | 32.736 | 1.00 | 0.00 |
| ATOM | 587 | H | LYS | 2 | 318 | 16.316 | 54.413 | 31.072 | 1.00 | 0.00 |
| ATOM | 588 | 1HZ | LYS | 2 | 318 | 11.321 | 59.224 | 33.269 | 1.00 | 0.00 |
| ATOM | 589 | 2HZ | LYS | 2 | 318 | 11.392 | 57.530 | 33.064 | 1.00 | 0.00 |
| ATOM | 590 | 3HZ | LYS | 2 | 318 | 12.771 | 58.472 | 32.989 | 1.00 | 0.00 |
| ATOM | 591 | N | THR | 2 | 319 | 14.008 | 55.589 | 33.710 | 1.00 | 0.00 |
| ATOM | 592 | CA | THR | 2 | 319 | 13.153 | 55.945 | 34.836 | 1.00 | 0.00 |
| ATOM | 593 | C | THR | 2 | 319 | 13.722 | 55.629 | 36.219 | 1.00 | 0.00 |
| ATOM | 594 | O | THR | 2 | 319 | 13.255 | 56.154 | 37.233 | 1.00 | 0.00 |
| ATOM | 595 | CB | THR | 2 | 319 | 11.744 | 55.403 | 34.554 | 1.00 | 0.00 |
| ATOM | 596 | OG1 | THR | 2 | 319 | 11.347 | 55.860 | 33.243 | 1.00 | 0.00 |
| ATOM | 597 | CG2 | THR | 2 | 319 | 10.680 | 55.835 | 35.569 | 1.00 | 0.00 |
| ATOM | 598 | H | THR | 2 | 319 | 14.268 | 54.637 | 33.532 | 1.00 | 0.00 |
| ATOM | 599 | HG1 | THR | 2 | 319 | 10.728 | 55.197 | 32.926 | 1.00 | 0.00 |
| ATOM | 600 | N | THR | 2 | 320 | 14.796 | 54.819 | 36.209 | 1.00 | 0.00 |
| ATOM | 601 | CA | THR | 2 | 320 | 15.556 | 54.692 | 37.454 | 1.00 | 0.00 |
| ATOM | 602 | C | THR | 2 | 320 | 16.167 | 56.006 | 37.932 | 1.00 | 0.00 |
| ATOM | 603 | O | THR | 2 | 320 | 16.116 | 56.391 | 39.095 | 1.00 | 0.00 |
| ATOM | 604 | CB | THR | 2 | 320 | 16.623 | 53.593 | 37.324 | 1.00 | 0.00 |
| ATOM | 605 | OG1 | THR | 2 | 320 | 17.427 | 53.771 | 36.147 | 1.00 | 0.00 |
| ATOM | 606 | CG2 | THR | 2 | 320 | 16.008 | 52.193 | 37.270 | 1.00 | 0.00 |
| ATOM | 607 | H | THR | 2 | 320 | 15.165 | 54.463 | 35.355 | 1.00 | 0.00 |
| ATOM | 608 | HG1 | THR | 2 | 320 | 17.030 | 53.203 | 35.486 | 1.00 | 0.00 |
| ATOM | 609 | N | ALA | 2 | 321 | 16.728 | 56.732 | 36.955 | 1.00 | 0.00 |
| ATOM | 610 | CA | ALA | 2 | 321 | 17.345 | 58.013 | 37.281 | 1.00 | 0.00 |
| ATOM | 611 | C | ALA | 2 | 321 | 16.616 | 59.203 | 36.681 | 1.00 | 0.00 |
| ATOM | 612 | O | ALA | 2 | 321 | 17.194 | 60.090 | 36.043 | 1.00 | 0.00 |
| ATOM | 613 | CB | ALA | 2 | 321 | 18.798 | 58.030 | 36.797 | 1.00 | 0.00 |
| ATOM | 614 | H | ALA | 2 | 321 | 16.790 | 56.351 | 36.034 | 1.00 | 0.00 |
| ATOM | 615 | N | ASP | 2 | 322 | 15.285 | 59.214 | 36.875 | 1.00 | 0.00 |
| ATOM | 616 | CA | ASP | 2 | 322 | 14.547 | 60.147 | 36.021 | 1.00 | 0.00 |
| ATOM | 617 | C | ASP | 2 | 322 | 14.819 | 61.646 | 36.170 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 618 | O | ASP | 2 | 322 | 14.493 | 62.314 | 37.155 | 1.00 | 0.00 |
| ATOM | 619 | CB | ASP | 2 | 322 | 13.044 | 59.848 | 36.016 | 1.00 | 0.00 |
| ATOM | 620 | CG | ASP | 2 | 322 | 12.373 | 60.438 | 34.778 | 1.00 | 0.00 |
| ATOM | 621 | OD1 | ASP | 2 | 322 | 11.158 | 60.374 | 34.676 | 1.00 | 0.00 |
| ATOM | 622 | OD2 | ASP | 2 | 322 | 13.048 | 60.950 | 33.889 | 1.00 | 0.00 |
| ATOM | 623 | H | ASP | 2 | 322 | 14.851 | 58.572 | 37.512 | 1.00 | 0.00 |
| ATOM | 624 | N | GLY | 2 | 323 | 15.418 | 62.163 | 35.092 | 1.00 | 0.00 |
| ATOM | 625 | CA | GLY | 2 | 323 | 15.722 | 63.593 | 35.089 | 1.00 | 0.00 |
| ATOM | 626 | C | GLY | 2 | 323 | 14.497 | 64.494 | 35.025 | 1.00 | 0.00 |
| ATOM | 627 | O | GLY | 2 | 323 | 14.512 | 65.655 | 35.437 | 1.00 | 0.00 |
| ATOM | 628 | H | GLY | 2 | 323 | 15.572 | 61.604 | 34.276 | 1.00 | 0.00 |
| ATOM | 629 | N | VAL | 2 | 324 | 13.407 | 63.895 | 34.527 | 1.00 | 0.00 |
| ATOM | 630 | CA | VAL | 2 | 324 | 12.107 | 64.571 | 34.547 | 1.00 | 0.00 |
| ATOM | 631 | C | VAL | 2 | 324 | 11.493 | 64.657 | 35.941 | 1.00 | 0.00 |
| ATOM | 632 | O | VAL | 2 | 324 | 10.646 | 65.505 | 36.240 | 1.00 | 0.00 |
| ATOM | 633 | CB | VAL | 2 | 324 | 11.111 | 63.874 | 33.598 | 1.00 | 0.00 |
| ATOM | 634 | CG1 | VAL | 2 | 324 | 9.868 | 64.729 | 33.325 | 1.00 | 0.00 |
| ATOM | 635 | CG2 | VAL | 2 | 324 | 11.761 | 63.444 | 32.286 | 1.00 | 0.00 |
| ATOM | 636 | H | VAL | 2 | 324 | 13.493 | 62.957 | 34.206 | 1.00 | 0.00 |
| ATOM | 637 | N | ALA | 2 | 325 | 11.923 | 63.697 | 36.776 | 1.00 | 0.00 |
| ATOM | 638 | CA | ALA | 2 | 325 | 11.170 | 63.458 | 37.999 | 1.00 | 0.00 |
| ATOM | 639 | C | ALA | 2 | 325 | 11.828 | 63.911 | 39.280 | 1.00 | 0.00 |
| ATOM | 640 | O | ALA | 2 | 325 | 11.234 | 64.669 | 40.034 | 1.00 | 0.00 |
| ATOM | 641 | CB | ALA | 2 | 325 | 10.794 | 61.981 | 38.130 | 1.00 | 0.00 |
| ATOM | 642 | H | ALA | 2 | 325 | 12.653 | 63.091 | 36.467 | 1.00 | 0.00 |
| ATOM | 643 | N | ARG | 2 | 326 | 13.069 | 63.419 | 39.528 | 1.00 | 0.00 |
| ATOM | 644 | CA | ARG | 2 | 326 | 13.628 | 63.717 | 40.860 | 1.00 | 0.00 |
| ATOM | 645 | C | ARG | 2 | 326 | 13.802 | 65.203 | 41.168 | 1.00 | 0.00 |
| ATOM | 646 | O | ARG | 2 | 326 | 13.385 | 65.721 | 42.197 | 1.00 | 0.00 |
| ATOM | 647 | CB | ARG | 2 | 326 | 14.915 | 62.934 | 41.164 | 1.00 | 0.00 |
| ATOM | 648 | CG | ARG | 2 | 326 | 14.752 | 61.413 | 41.324 | 1.00 | 0.00 |
| ATOM | 649 | CD | ARG | 2 | 326 | 16.026 | 60.739 | 41.865 | 1.00 | 0.00 |
| ATOM | 650 | NE | ARG | 2 | 326 | 15.909 | 59.280 | 41.926 | 1.00 | 0.00 |
| ATOM | 651 | CZ | ARG | 2 | 326 | 16.934 | 58.452 | 41.611 | 1.00 | 0.00 |
| ATOM | 652 | NH1 | ARG | 2 | 326 | 16.740 | 57.145 | 41.593 | 1.00 | 0.00 |
| ATOM | 653 | NH2 | ARG | 2 | 326 | 18.129 | 58.926 | 41.279 | 1.00 | 0.00 |
| ATOM | 654 | H | ARG | 2 | 326 | 13.600 | 62.961 | 38.812 | 1.00 | 0.00 |
| ATOM | 655 | HE | ARG | 2 | 326 | 15.063 | 58.850 | 42.268 | 1.00 | 0.00 |
| ATOM | 656 | 1HH1 | ARG | 2 | 326 | 17.455 | 56.515 | 41.252 | 1.00 | 0.00 |
| ATOM | 657 | 2HH1 | ARG | 2 | 326 | 15.860 | 56.766 | 41.895 | 1.00 | 0.00 |
| ATOM | 658 | 1HH2 | ARG | 2 | 326 | 18.838 | 58.286 | 40.944 | 1.00 | 0.00 |
| ATOM | 659 | 2HH2 | ARG | 2 | 326 | 18.345 | 59.898 | 41.371 | 1.00 | 0.00 |
| ATOM | 660 | N | VAL | 2 | 327 | 14.348 | 65.905 | 40.176 | 1.00 | 0.00 |
| ATOM | 661 | CA | VAL | 2 | 327 | 14.456 | 67.354 | 40.341 | 1.00 | 0.00 |
| ATOM | 662 | C | VAL | 2 | 327 | 13.112 | 68.081 | 40.447 | 1.00 | 0.00 |
| ATOM | 663 | O | VAL | 2 | 327 | 12.989 | 69.177 | 40.993 | 1.00 | 0.00 |
| ATOM | 664 | CB | VAL | 2 | 327 | 15.329 | 67.926 | 39.218 | 1.00 | 0.00 |
| ATOM | 665 | CG1 | VAL | 2 | 327 | 15.635 | 69.402 | 39.452 | 1.00 | 0.00 |
| ATOM | 666 | CG2 | VAL | 2 | 327 | 16.624 | 67.125 | 39.067 | 1.00 | 0.00 |
| ATOM | 667 | H | VAL | 2 | 327 | 14.696 | 65.420 | 39.377 | 1.00 | 0.00 |
| ATOM | 668 | N | ARG | 2 | 328 | 12.101 | 67.422 | 39.878 | 1.00 | 0.00 |
| ATOM | 669 | CA | ARG | 2 | 328 | 10.750 | 67.952 | 40.004 | 1.00 | 0.00 |
| ATOM | 670 | C | ARG | 2 | 328 | 10.004 | 67.434 | 41.228 | 1.00 | 0.00 |
| ATOM | 671 | O | ARG | 2 | 328 | 8.860 | 67.802 | 41.500 | 1.00 | 0.00 |
| ATOM | 672 | CB | ARG | 2 | 328 | 9.986 | 67.679 | 38.711 | 1.00 | 0.00 |
| ATOM | 673 | CG | ARG | 2 | 328 | 8.828 | 68.650 | 38.518 | 1.00 | 0.00 |
| ATOM | 674 | CD | ARG | 2 | 328 | 7.971 | 68.337 | 37.301 | 1.00 | 0.00 |
| ATOM | 675 | NE | ARG | 2 | 328 | 6.869 | 69.292 | 37.251 | 1.00 | 0.00 |
| ATOM | 676 | CZ | ARG | 2 | 328 | 5.584 | 68.889 | 37.148 | 1.00 | 0.00 |
| ATOM | 677 | NH1 | ARG | 2 | 328 | 4.610 | 69.793 | 37.117 | 1.00 | 0.00 |
| ATOM | 678 | NH2 | ARG | 2 | 328 | 5.293 | 67.593 | 37.060 | 1.00 | 0.00 |
| ATOM | 679 | H | ARG | 2 | 328 | 12.230 | 66.487 | 39.553 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 680 | HE | ARG | 2 | 328 | 7.127 | 70.260 | 37.344 | 1.00 | 0.00 |
| ATOM | 681 | 1HH1 | ARG | 2 | 328 | 3.658 | 69.531 | 36.952 | 1.00 | 0.00 |
| ATOM | 682 | 2HH1 | ARG | 2 | 328 | 4.818 | 70.760 | 37.255 | 1.00 | 0.00 |
| ATOM | 683 | 1HH2 | ARG | 2 | 328 | 4.355 | 67.290 | 36.890 | 1.00 | 0.00 |
| ATOM | 684 | 2HH2 | ARG | 2 | 328 | 6.015 | 66.903 | 37.159 | 1.00 | 0.00 |
| ATOM | 685 | N | LYS | 2 | 329 | 10.712 | 66.552 | 41.965 | 1.00 | 0.00 |
| ATOM | 686 | CA | LYS | 2 | 329 | 10.343 | 66.306 | 43.355 | 1.00 | 0.00 |
| ATOM | 687 | C | LYS | 2 | 329 | 10.767 | 37.505 | 44.185 | 1.00 | 0.00 |
| ATOM | 688 | O | LYS | 2 | 329 | 9.981 | 68.069 | 44.938 | 1.00 | 0.00 |
| ATOM | 689 | CB | LYS | 2 | 329 | 11.017 | 65.065 | 43.985 | 1.00 | 0.00 |
| ATOM | 690 | CG | LYS | 2 | 329 | 10.812 | 63.643 | 43.435 | 1.00 | 0.00 |
| ATOM | 691 | CD | LYS | 2 | 329 | 11.696 | 62.629 | 44.199 | 1.00 | 0.00 |
| ATOM | 692 | CE | LYS | 2 | 329 | 11.544 | 61.156 | 43.774 | 1.00 | 0.00 |
| ATOM | 693 | NZ | LYS | 2 | 329 | 12.435 | 60.265 | 44.536 | 1.00 | 0.00 |
| ATOM | 694 | H | LYS | 2 | 329 | 11.569 | 66.208 | 41.592 | 1.00 | 0.00 |
| ATOM | 695 | 1HZ | LYS | 2 | 329 | 12.209 | 59.272 | 44.318 | 1.00 | 0.00 |
| ATOM | 696 | 2HZ | LYS | 2 | 329 | 13.429 | 60.336 | 44.257 | 1.00 | 0.00 |
| ATOM | 697 | 3HZ | LYS | 2 | 329 | 12.334 | 60.419 | 45.557 | 1.00 | 0.00 |
| ATOM | 698 | N | SER | 2 | 330 | 12.051 | 67.878 | 44.067 | 1.00 | 0.00 |
| ATOM | 699 | CA | SER | 2 | 330 | 12.451 | 68.765 | 45.158 | 1.00 | 0.00 |
| ATOM | 700 | C | SER | 2 | 330 | 13.141 | 70.058 | 44.802 | 1.00 | 0.00 |
| ATOM | 701 | O | SER | 2 | 330 | 14.362 | 70.108 | 44.769 | 1.00 | 0.00 |
| ATOM | 702 | CB | SER | 2 | 330 | 13.271 | 67.991 | 46.194 | 1.00 | 0.00 |
| ATOM | 703 | OG | SER | 2 | 330 | 13.142 | 66.579 | 45.934 | 1.00 | 0.00 |
| ATOM | 704 | H | SER | 2 | 330 | 12.684 | 67.428 | 43.436 | 1.00 | 0.00 |
| ATOM | 705 | HG | SER | 2 | 330 | 13.928 | 66.282 | 45.459 | 1.00 | 0.00 |
| ATOM | 706 | N | LYS | 2 | 331 | 12.312 | 71.100 | 44.585 | 1.00 | 0.00 |
| ATOM | 707 | CA | LYS | 2 | 331 | 12.703 | 72.510 | 44.794 | 1.00 | 0.00 |
| ATOM | 708 | C | LYS | 2 | 331 | 14.192 | 72.881 | 44.929 | 1.00 | 0.00 |
| ATOM | 709 | O | LYS | 2 | 331 | 14.751 | 72.833 | 46.024 | 1.00 | 0.00 |
| ATOM | 710 | CB | LYS | 2 | 331 | 11.923 | 72.991 | 46.025 | 1.00 | 0.00 |
| ATOM | 711 | CG | LYS | 2 | 331 | 12.034 | 74.464 | 46.428 | 1.00 | 0.00 |
| ATOM | 712 | CD | LYS | 2 | 331 | 11.485 | 74.648 | 47.844 | 1.00 | 0.00 |
| ATOM | 713 | CE | LYS | 2 | 331 | 11.626 | 76.066 | 48.398 | 1.00 | 0.00 |
| ATOM | 714 | NZ | LYS | 2 | 331 | 11.188 | 76.064 | 49.796 | 1.00 | 0.00 |
| ATOM | 715 | H | LYS | 2 | 331 | 11.353 | 70.845 | 44.465 | 1.00 | 0.00 |
| ATOM | 716 | 1HZ | LYS | 2 | 331 | 11.139 | 77.040 | 50.148 | 1.00 | 0.00 |
| ATOM | 717 | 2HZ | LYS | 2 | 331 | 10.253 | 75.620 | 49.844 | 1.00 | 0.00 |
| ATOM | 718 | 3HZ | LYS | 2 | 331 | 11.842 | 75.508 | 50.381 | 1.00 | 0.00 |
| ATOM | 719 | N | GLY | 2 | 332 | 14.772 | 73.300 | 43.789 | 1.00 | 0.00 |
| ATOM | 720 | CA | GLY | 2 | 332 | 16.201 | 73.616 | 43.818 | 1.00 | 0.00 |
| ATOM | 721 | C | GLY | 2 | 332 | 16.985 | 72.335 | 43.981 | 1.00 | 0.00 |
| ATOM | 722 | O | GLY | 2 | 332 | 16.695 | 71.359 | 43.298 | 1.00 | 0.00 |
| ATOM | 723 | H | GLY | 2 | 332 | 14.255 | 73.297 | 42.941 | 1.00 | 0.00 |
| ATOM | 724 | N | LYS | 2 | 333 | 17.895 | 72.394 | 44.958 | 1.00 | 0.00 |
| ATOM | 725 | CA | LYS | 2 | 333 | 18.462 | 71.249 | 45.682 | 1.00 | 0.00 |
| ATOM | 726 | C | LYS | 2 | 333 | 18.814 | 69.945 | 44.980 | 1.00 | 0.00 |
| ATOM | 727 | O | LYS | 2 | 333 | 19.990 | 69.587 | 44.893 | 1.00 | 0.00 |
| ATOM | 728 | CB | LYS | 2 | 333 | 17.621 | 70.975 | 46.927 | 1.00 | 0.00 |
| ATOM | 729 | CG | LYS | 2 | 333 | 17.973 | 71.948 | 48.048 | 1.00 | 0.00 |
| ATOM | 730 | CD | LYS | 2 | 333 | 17.065 | 71.797 | 49.266 | 1.00 | 0.00 |
| ATOM | 731 | CE | LYS | 2 | 333 | 17.724 | 72.333 | 50.538 | 1.00 | 0.00 |
| ATOM | 732 | NZ | LYS | 2 | 333 | 18.867 | 71.482 | 50.880 | 1.00 | 0.00 |
| ATOM | 733 | H | LYS | 2 | 333 | 18.084 | 73.325 | 45.252 | 1.00 | 0.00 |
| ATOM | 734 | 1HZ | LYS | 2 | 333 | 18.540 | 70.547 | 51.202 | 1.00 | 0.00 |
| ATOM | 735 | 2HZ | LYS | 2 | 333 | 19.458 | 71.265 | 50.054 | 1.00 | 0.00 |
| ATOM | 736 | 3HZ | LYS | 2 | 333 | 19.481 | 71.920 | 51.597 | 1.00 | 0.00 |
| ATOM | 737 | N | PHE | 2 | 334 | 17.750 | 69.248 | 44.552 | 1.00 | 0.00 |
| ATOM | 738 | CA | PHE | 2 | 334 | 17.900 | 67.995 | 43.812 | 1.00 | 0.00 |
| ATOM | 739 | C | PHE | 2 | 334 | 18.564 | 68.234 | 42.483 | 1.00 | 0.00 |
| ATOM | 740 | O | PHE | 2 | 334 | 18.353 | 69.292 | 41.866 | 1.00 | 0.00 |
| ATOM | 741 | CB | PHE | 2 | 334 | 16.535 | 67.332 | 43.611 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 742 | CG | PHE | 2 | 334 | 16.312 | 66.216 | 44.607 | 1.00 | 0.00 |
| ATOM | 743 | CD1 | PHE | 2 | 334 | 15.964 | 64.939 | 44.117 | 1.00 | 0.00 |
| ATOM | 744 | CD2 | PHE | 2 | 334 | 16.437 | 66.452 | 45.995 | 1.00 | 0.00 |
| ATOM | 745 | CE1 | PHE | 2 | 334 | 15.735 | 63.884 | 45.021 | 1.00 | 0.00 |
| ATOM | 746 | CE2 | PHE | 2 | 334 | 16.210 | 65.399 | 46.902 | 1.00 | 0.00 |
| ATOM | 747 | CZ | PHE | 2 | 334 | 15.860 | 64.126 | 46.405 | 1.00 | 0.00 |
| ATOM | 748 | H | PHE | 2 | 334 | 16.899 | 69.767 | 44.511 | 1.00 | 0.00 |
| ATOM | 749 | N | ALA | 2 | 335 | 19.402 | 67.242 | 42.152 | 1.00 | 0.00 |
| ATOM | 750 | CA | ALA | 2 | 335 | 20.390 | 67.332 | 41.093 | 1.00 | 0.00 |
| ATOM | 751 | C | ALA | 2 | 335 | 21.011 | 65.997 | 40.738 | 1.00 | 0.00 |
| ATOM | 752 | O | ALA | 2 | 335 | 21.601 | 65.329 | 41.591 | 1.00 | 0.00 |
| ATOM | 753 | CB | ALA | 2 | 335 | 21.527 | 68.271 | 41.499 | 1.00 | 0.00 |
| ATOM | 754 | H | ALA | 2 | 335 | 19.355 | 66.401 | 42.678 | 1.00 | 0.00 |
| ATOM | 755 | N | PHE | 2 | 336 | 20.927 | 65.679 | 39.434 | 1.00 | 0.00 |
| ATOM | 756 | CA | PHE | 2 | 336 | 21.722 | 64.597 | 38.836 | 1.00 | 0.00 |
| ATOM | 757 | C | PHE | 2 | 336 | 23.025 | 65.064 | 38.209 | 1.00 | 0.00 |
| ATOM | 758 | O | PHE | 2 | 336 | 23.268 | 66.259 | 38.030 | 1.00 | 0.00 |
| ATOM | 759 | CB | PHE | 2 | 336 | 20.982 | 63.866 | 37.717 | 1.00 | 0.00 |
| ATOM | 760 | CG | PHE | 2 | 336 | 19.753 | 63.135 | 38.180 | 1.00 | 0.00 |
| ATOM | 761 | CD1 | PHE | 2 | 336 | 19.877 | 61.800 | 38.617 | 1.00 | 0.00 |
| ATOM | 762 | CD2 | PHE | 2 | 336 | 18.503 | 63.786 | 38.127 | 1.00 | 0.00 |
| ATOM | 763 | CE1 | PHE | 2 | 336 | 18.718 | 61.086 | 38.966 | 1.00 | 0.00 |
| ATOM | 764 | CE2 | PHE | 2 | 336 | 17.344 | 63.071 | 38.477 | 1.00 | 0.00 |
| ATOM | 765 | CZ | PHE | 2 | 336 | 17.464 | 61.723 | 38.871 | 1.00 | 0.00 |
| ATOM | 766 | H | PHE | 2 | 336 | 20.301 | 66.263 | 38.925 | 1.00 | 0.00 |
| ATOM | 767 | N | LEU | 2 | 337 | 23.842 | 64.040 | 37.890 | 1.00 | 0.00 |
| ATOM | 768 | CA | LEU | 2 | 337 | 25.119 | 64.104 | 37.169 | 1.00 | 0.00 |
| ATOM | 769 | C | LEU | 2 | 337 | 25.181 | 62.931 | 36.186 | 1.00 | 0.00 |
| ATOM | 770 | O | LEU | 2 | 337 | 25.301 | 61.768 | 36.555 | 1.00 | 0.00 |
| ATOM | 771 | CB | LEU | 2 | 337 | 26.312 | 63.953 | 38.128 | 1.00 | 0.00 |
| ATOM | 772 | CG | LEU | 2 | 337 | 26.806 | 65.117 | 39.004 | 1.00 | 0.00 |
| ATOM | 773 | CD1 | LEU | 2 | 337 | 25.811 | 65.638 | 40.042 | 1.00 | 0.00 |
| ATOM | 774 | CD2 | LEU | 2 | 337 | 28.105 | 64.714 | 39.704 | 1.00 | 0.00 |
| ATOM | 775 | H | LEU | 2 | 337 | 23.545 | 63.170 | 38.276 | 1.00 | 0.00 |
| ATOM | 776 | N | LEU | 2 | 338 | 25.027 | 63.224 | 34.899 | 1.00 | 0.00 |
| ATOM | 777 | CA | LEU | 2 | 338 | 25.401 | 62.152 | 33.963 | 1.00 | 0.00 |
| ATOM | 778 | C | LEU | 2 | 338 | 26.498 | 62.704 | 33.099 | 1.00 | 0.00 |
| ATOM | 779 | O | LEU | 2 | 338 | 26.552 | 63.923 | 32.925 | 1.00 | 0.00 |
| ATOM | 780 | CB | LEU | 2 | 338 | 24.239 | 61.707 | 33.070 | 1.00 | 0.00 |
| ATOM | 781 | CG | LEU | 2 | 338 | 23.366 | 60.571 | 33.615 | 1.00 | 0.00 |
| ATOM | 782 | CD1 | LEU | 2 | 338 | 22.558 | 60.950 | 34.858 | 1.00 | 0.00 |
| ATOM | 783 | CD2 | LEU | 2 | 338 | 22.472 | 59.996 | 32.516 | 1.00 | 0.00 |
| ATOM | 784 | H | LEU | 2 | 338 | 24.935 | 64.182 | 34.618 | 1.00 | 0.00 |
| ATOM | 785 | N | GLU | 2 | 339 | 27.366 | 61.830 | 32.569 | 1.00 | 0.00 |
| ATOM | 786 | CA | GLU | 2 | 339 | 28.278 | 62.294 | 31.518 | 1.00 | 0.00 |
| ATOM | 787 | C | GLU | 2 | 339 | 27.458 | 62.657 | 30.276 | 1.00 | 0.00 |
| ATOM | 788 | O | GLU | 2 | 339 | 26.311 | 62.219 | 30.166 | 1.00 | 0.00 |
| ATOM | 789 | CB | GLU | 2 | 339 | 29.402 | 61.258 | 31.257 | 1.00 | 0.00 |
| ATOM | 790 | CG | GLU | 2 | 339 | 30.178 | 60.783 | 32.513 | 1.00 | 0.00 |
| ATOM | 791 | CD | GLU | 2 | 339 | 31.545 | 60.163 | 32.185 | 1.00 | 0.00 |
| ATOM | 792 | OE1 | GLU | 2 | 339 | 32.289 | 60.724 | 31.416 | 1.00 | 0.00 |
| ATOM | 793 | OE2 | GLU | 2 | 339 | 31.930 | 59.125 | 32.701 | 1.00 | 0.00 |
| ATOM | 794 | H | GLU | 2 | 339 | 27.151 | 60.892 | 32.812 | 1.00 | 0.00 |
| ATOM | 795 | N | SER | 2 | 340 | 28.030 | 63.522 | 29.420 | 1.00 | 0.00 |
| ATOM | 796 | CA | SER | 2 | 340 | 27.339 | 63.926 | 28.189 | 1.00 | 0.00 |
| ATOM | 797 | C | SER | 2 | 340 | 25.852 | 64.282 | 28.219 | 1.00 | 0.00 |
| ATOM | 798 | O | SER | 2 | 340 | 25.486 | 65.455 | 28.329 | 1.00 | 0.00 |
| ATOM | 799 | CB | SER | 2 | 340 | 27.659 | 62.967 | 27.042 | 1.00 | 0.00 |
| ATOM | 800 | OG | SER | 2 | 340 | 28.962 | 63.233 | 26.501 | 1.00 | 0.00 |
| ATOM | 801 | H | SER | 2 | 340 | 29.007 | 63.684 | 29.505 | 1.00 | 0.00 |
| ATOM | 802 | HG | SER | 2 | 340 | 28.843 | 63.160 | 25.556 | 1.00 | 0.00 |
| ATOM | 803 | N | THR | 2 | 341 | 24.978 | 63.278 | 28.100 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 804 | CA | THR | 2 | 341 | 23.580 | 63.565 | 27.771 | 1.00 | 0.00 |
| ATOM | 805 | C | THR | 2 | 341 | 22.650 | 64.065 | 28.864 | 1.00 | 0.00 |
| ATOM | 806 | O | THR | 2 | 341 | 21.419 | 64.079 | 28.756 | 1.00 | 0.00 |
| ATOM | 807 | CB | THR | 2 | 341 | 22.953 | 62.395 | 27.031 | 1.00 | 0.00 |
| ATOM | 808 | OG1 | THR | 2 | 341 | 23.884 | 61.306 | 26.887 | 1.00 | 0.00 |
| ATOM | 809 | CG2 | THR | 2 | 341 | 22.509 | 62.846 | 25.646 | 1.00 | 0.00 |
| ATOM | 810 | H | THR | 2 | 341 | 25.336 | 62.364 | 28.282 | 1.00 | 0.00 |
| ATOM | 811 | HG1 | THR | 2 | 341 | 24.036 | 60.974 | 27.775 | 1.00 | 0.00 |
| ATOM | 812 | N | MET | 2 | 342 | 23.274 | 64.520 | 29.960 | 1.00 | 0.00 |
| ATOM | 813 | CA | MET | 2 | 342 | 22.406 | 65.251 | 30.875 | 1.00 | 0.00 |
| ATOM | 814 | C | MET | 2 | 342 | 21.980 | 66.642 | 30.420 | 1.00 | 0.00 |
| ATOM | 815 | O | MET | 2 | 342 | 21.124 | 67.284 | 31.026 | 1.00 | 0.00 |
| ATOM | 816 | CB | MET | 2 | 342 | 22.933 | 65.196 | 32.306 | 1.00 | 0.00 |
| ATOM | 817 | CG | MET | 2 | 342 | 21.811 | 64.790 | 33.265 | 1.00 | 0.00 |
| ATOM | 818 | SD | MET | 2 | 342 | 20.958 | 63.292 | 32.731 | 1.00 | 0.00 |
| ATOM | 819 | CE | MET | 2 | 342 | 19.742 | 63.174 | 34.055 | 1.00 | 0.00 |
| ATOM | 820 | H | MET | 2 | 342 | 24.261 | 64.430 | 30.080 | 1.00 | 0.00 |
| ATOM | 821 | N | ASN | 2 | 343 | 22.569 | 67.039 | 29.282 | 1.00 | 0.00 |
| ATOM | 822 | CA | ASN | 2 | 343 | 21.862 | 68.029 | 28.480 | 1.00 | 0.00 |
| ATOM | 823 | C | ASN | 2 | 343 | 20.884 | 67.327 | 27.541 | 1.00 | 0.00 |
| ATOM | 824 | O | ASN | 2 | 343 | 20.080 | 66.546 | 28.036 | 1.00 | 0.00 |
| ATOM | 825 | CB | ASN | 2 | 343 | 22.825 | 69.030 | 27.827 | 1.00 | 0.00 |
| ATOM | 826 | CG | ASN | 2 | 343 | 22.153 | 70.390 | 27.873 | 1.00 | 0.00 |
| ATOM | 827 | OD1 | ASN | 2 | 343 | 21.564 | 70.775 | 28.884 | 1.00 | 0.00 |
| ATOM | 828 | ND2 | ASN | 2 | 343 | 22.203 | 71.084 | 26.737 | 1.00 | 0.00 |
| ATOM | 829 | H | ASN | 2 | 343 | 23.290 | 66.490 | 28.864 | 1.00 | 0.00 |
| ATOM | 830 | 1HD2 | ASN | 2 | 343 | 21.683 | 71.942 | 26.664 | 1.00 | 0.00 |
| ATOM | 831 | 2HD2 | ASN | 2 | 343 | 22.700 | 70.797 | 25.919 | 1.00 | 0.00 |
| ATOM | 832 | N | GLU | 2 | 344 | 20.941 | 67.568 | 26.217 | 1.00 | 0.00 |
| ATOM | 833 | CA | GLU | 2 | 344 | 19.975 | 67.015 | 25.246 | 1.00 | 0.00 |
| ATOM | 834 | C | GLU | 2 | 344 | 19.042 | 65.847 | 25.587 | 1.00 | 0.00 |
| ATOM | 835 | O | GLU | 2 | 344 | 17.832 | 65.975 | 25.446 | 1.00 | 0.00 |
| ATOM | 836 | CB | GLU | 2 | 344 | 20.617 | 66.803 | 23.865 | 1.00 | 0.00 |
| ATOM | 837 | CG | GLU | 2 | 344 | 21.841 | 65.879 | 23.801 | 1.00 | 0.00 |
| ATOM | 838 | CD | GLU | 2 | 344 | 23.004 | 66.527 | 24.520 | 1.00 | 0.00 |
| ATOM | 839 | OE1 | GLU | 2 | 344 | 23.478 | 67.545 | 24.056 | 1.00 | 0.00 |
| ATOM | 840 | OE2 | GLU | 2 | 344 | 23.418 | 66.052 | 25.566 | 1.00 | 0.00 |
| ATOM | 841 | H | GLU | 2 | 344 | 21.628 | 68.212 | 25.889 | 1.00 | 0.00 |
| ATOM | 842 | N | TYR | 2 | 345 | 19.571 | 64.706 | 26.069 | 1.00 | 0.00 |
| ATOM | 843 | CA | TYR | 2 | 345 | 18.632 | 63.630 | 26.446 | 1.00 | 0.00 |
| ATOM | 844 | C | TYR | 2 | 345 | 17.593 | 64.068 | 27.467 | 1.00 | 0.00 |
| ATOM | 845 | O | TYR | 2 | 345 | 16.387 | 63.823 | 27.367 | 1.00 | 0.00 |
| ATOM | 846 | CB | TYR | 2 | 345 | 19.384 | 62.416 | 26.999 | 1.00 | 0.00 |
| ATOM | 847 | CG | TYR | 2 | 345 | 18.598 | 61.124 | 27.010 | 1.00 | 0.00 |
| ATOM | 848 | CD1 | TYR | 2 | 345 | 18.522 | 60.362 | 25.827 | 1.00 | 0.00 |
| ATOM | 849 | CD2 | TYR | 2 | 345 | 18.005 | 60.691 | 28.213 | 1.00 | 0.00 |
| ATOM | 850 | CE1 | TYR | 2 | 345 | 17.880 | 59.113 | 25.858 | 1.00 | 0.00 |
| ATOM | 851 | CE2 | TYR | 2 | 345 | 17.363 | 59.441 | 28.245 | 1.00 | 0.00 |
| ATOM | 852 | CZ | TYR | 2 | 345 | 17.321 | 58.661 | 27.070 | 1.00 | 0.00 |
| ATOM | 853 | OH | TYR | 2 | 345 | 16.707 | 57.420 | 27.102 | 1.00 | 0.00 |
| ATOM | 854 | H | TYR | 2 | 345 | 20.567 | 64.640 | 26.158 | 1.00 | 0.00 |
| ATOM | 855 | HH | TYR | 2 | 345 | 16.373 | 57.294 | 27.989 | 1.00 | 0.00 |
| ATOM | 856 | N | ILE | 2 | 346 | 18.121 | 64.744 | 28.490 | 1.00 | 0.00 |
| ATOM | 857 | CA | ILE | 2 | 346 | 17.211 | 65.223 | 29.511 | 1.00 | 0.00 |
| ATOM | 858 | C | ILE | 2 | 346 | 16.862 | 66.706 | 29.461 | 1.00 | 0.00 |
| ATOM | 859 | O | ILE | 2 | 346 | 15.992 | 67.162 | 30.192 | 1.00 | 0.00 |
| ATOM | 860 | CB | ILE | 2 | 346 | 17.673 | 64.734 | 30.894 | 1.00 | 0.00 |
| ATOM | 861 | CG1 | ILE | 2 | 346 | 16.479 | 64.184 | 31.666 | 1.00 | 0.00 |
| ATOM | 862 | CG2 | ILE | 2 | 346 | 18.400 | 65.815 | 31.705 | 1.00 | 0.00 |
| ATOM | 863 | CD1 | ILE | 2 | 346 | 15.935 | 62.881 | 31.075 | 1.00 | 0.00 |
| ATOM | 864 | H | ILE | 2 | 346 | 19.079 | 65.030 | 28.433 | 1.00 | 0.00 |
| ATOM | 865 | N | GLU | 2 | 347 | 17.533 | 67.453 | 28.569 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 866 | CA | GLU | 2 | 347 | 17.327 | 68.904 | 28.569 | 1.00 | 0.00 |
| ATOM | 867 | C | GLU | 2 | 347 | 15.880 | 69.283 | 28.342 | 1.00 | 0.00 |
| ATOM | 868 | O | GLU | 2 | 347 | 15.197 | 69.823 | 29.214 | 1.00 | 0.00 |
| ATOM | 869 | CB | GLU | 2 | 347 | 18.234 | 69.594 | 27.548 | 1.00 | 0.00 |
| ATOM | 870 | CG | GLU | 2 | 347 | 18.669 | 71.023 | 27.899 | 1.00 | 0.00 |
| ATOM | 871 | CD | GLU | 2 | 347 | 17.505 | 71.971 | 28.073 | 1.00 | 0.00 |
| ATOM | 872 | OE1 | GLU | 2 | 347 | 17.453 | 72.655 | 29.092 | 1.00 | 0.00 |
| ATOM | 873 | OE2 | GLU | 2 | 347 | 16.649 | 72.023 | 27.199 | 1.00 | 0.00 |
| ATOM | 874 | H | GLU | 2 | 347 | 18.200 | 67.041 | 27.947 | 1.00 | 0.00 |
| ATOM | 875 | N | GLN | 2 | 348 | 15.418 | 68.873 | 27.158 | 1.00 | 0.00 |
| ATOM | 876 | CA | GLN | 2 | 348 | 14.009 | 69.098 | 26.860 | 1.00 | 0.00 |
| ATOM | 877 | C | GLN | 2 | 348 | 13.065 | 68.164 | 27.610 | 1.00 | 0.00 |
| ATOM | 878 | O | GLN | 2 | 348 | 11.843 | 68.218 | 27.502 | 1.00 | 0.00 |
| ATOM | 879 | CB | GLN | 2 | 348 | 13.722 | 69.089 | 25.352 | 1.00 | 0.00 |
| ATOM | 880 | CG | GLN | 2 | 348 | 14.756 | 69.780 | 24.449 | 1.00 | 0.00 |
| ATOM | 881 | CD | GLN | 2 | 348 | 15.961 | 68.878 | 24.259 | 1.00 | 0.00 |
| ATOM | 882 | OE1 | GLN | 2 | 348 | 15.855 | 67.653 | 24.171 | 1.00 | 0.00 |
| ATOM | 883 | NE2 | GLN | 2 | 348 | 17.138 | 69.516 | 24.252 | 1.00 | 0.00 |
| ATOM | 884 | H | GLN | 2 | 348 | 16.055 | 68.388 | 26.562 | 1.00 | 0.00 |
| ATOM | 885 | 1HE2 | GLN | 2 | 348 | 18.030 | 69.059 | 24.214 | 1.00 | 0.00 |
| ATOM | 886 | 2HE2 | GLN | 2 | 348 | 17.173 | 70.516 | 24.306 | 1.00 | 0.00 |
| ATOM | 887 | N | ARG | 2 | 349 | 13.662 | 67.247 | 28.420 | 1.00 | 0.00 |
| ATOM | 888 | CA | ARG | 2 | 349 | 12.831 | 66.560 | 29.378 | 1.00 | 0.00 |
| ATOM | 889 | C | ARG | 2 | 349 | 12.741 | 67.247 | 30.742 | 1.00 | 0.00 |
| ATOM | 890 | O | ARG | 2 | 349 | 12.228 | 66.711 | 31.724 | 1.00 | 0.00 |
| ATOM | 891 | CB | ARG | 2 | 349 | 13.275 | 65.100 | 29.447 | 1.00 | 0.00 |
| ATOM | 892 | CG | ARG | 2 | 349 | 12.424 | 64.145 | 28.592 | 1.00 | 0.00 |
| ATOM | 893 | CD | ARG | 2 | 349 | 12.406 | 64.423 | 27.084 | 1.00 | 0.00 |
| ATOM | 894 | NE | ARG | 2 | 349 | 13.753 | 64.342 | 26.525 | 1.00 | 0.00 |
| ATOM | 895 | CZ | ARG | 2 | 349 | 14.129 | 65.091 | 25.463 | 1.00 | 0.00 |
| ATOM | 896 | NH1 | ARG | 2 | 349 | 15.391 | 65.051 | 25.084 | 1.00 | 0.00 |
| ATOM | 897 | NH2 | ARG | 2 | 349 | 13.271 | 65.872 | 24.813 | 1.00 | 0.00 |
| ATOM | 898 | H | ARG | 2 | 349 | 14.655 | 67.328 | 28.536 | 1.00 | 0.00 |
| ATOM | 899 | HE | ARG | 2 | 349 | 14.424 | 63.690 | 26.892 | 1.00 | 0.00 |
| ATOM | 900 | 1HH1 | ARG | 2 | 349 | 16.004 | 64.384 | 25.521 | 1.00 | 0.00 |
| ATOM | 901 | 2HH1 | ARG | 2 | 349 | 15.784 | 65.683 | 24.409 | 1.00 | 0.00 |
| ATOM | 902 | 1HH2 | ARG | 2 | 349 | 13.552 | 66.405 | 24.008 | 1.00 | 0.00 |
| ATOM | 903 | 2HH2 | ARG | 2 | 349 | 12.322 | 65.925 | 25.119 | 1.00 | 0.00 |
| ATOM | 904 | N | LYS | 2 | 350 | 13.188 | 68.512 | 30.699 | 1.00 | 0.00 |
| ATOM | 905 | CA | LYS | 2 | 350 | 12.946 | 69.560 | 31.694 | 1.00 | 0.00 |
| ATOM | 906 | C | LYS | 2 | 350 | 13.360 | 70.929 | 31.136 | 1.00 | 0.00 |
| ATOM | 907 | O | LYS | 2 | 350 | 14.234 | 71.590 | 31.693 | 1.00 | 0.00 |
| ATOM | 908 | CB | LYS | 2 | 350 | 13.715 | 69.239 | 32.997 | 1.00 | 0.00 |
| ATOM | 909 | CG | LYS | 2 | 350 | 15.182 | 68.796 | 32.818 | 1.00 | 0.00 |
| ATOM | 910 | CD | LYS | 2 | 350 | 16.245 | 69.824 | 33.229 | 1.00 | 0.00 |
| ATOM | 911 | CE | LYS | 2 | 350 | 17.263 | 70.169 | 32.131 | 1.00 | 0.00 |
| ATOM | 912 | NZ | LYS | 2 | 350 | 16.661 | 71.009 | 31.083 | 1.00 | 0.00 |
| ATOM | 913 | H | LYS | 2 | 350 | 13.742 | 68.777 | 29.912 | 1.00 | 0.00 |
| ATOM | 914 | 1HZ | LYS | 2 | 350 | 17.343 | 71.465 | 30.438 | 1.00 | 0.00 |
| ATOM | 915 | 2HZ | LYS | 2 | 350 | 16.027 | 70.467 | 30.473 | 1.00 | 0.00 |
| ATOM | 916 | 3HZ | LYS | 2 | 350 | 16.076 | 71.758 | 31.504 | 1.00 | 0.00 |
| ATOM | 917 | N | PRO | 2 | 351 | 12.765 | 71.335 | 29.980 | 1.00 | 0.00 |
| ATOM | 918 | CA | PRO | 2 | 351 | 13.463 | 72.323 | 29.132 | 1.00 | 0.00 |
| ATOM | 919 | C | PRO | 2 | 351 | 13.709 | 73.643 | 29.835 | 1.00 | 0.00 |
| ATOM | 920 | O | PRO | 2 | 351 | 12.762 | 74.309 | 30.235 | 1.00 | 0.00 |
| ATOM | 921 | CB | PRO | 2 | 351 | 12.546 | 72.421 | 27.907 | 1.00 | 0.00 |
| ATOM | 922 | CG | PRO | 2 | 351 | 11.164 | 71.968 | 28.381 | 1.00 | 0.00 |
| ATOM | 923 | CD | PRO | 2 | 351 | 11.487 | 70.905 | 29.422 | 1.00 | 0.00 |
| ATOM | 924 | N | CYS | 2 | 352 | 15.010 | 73.934 | 30.032 | 1.00 | 0.00 |
| ATOM | 925 | CA | CYS | 2 | 352 | 15.599 | 74.983 | 30.886 | 1.00 | 0.00 |
| ATOM | 926 | C | CYS | 2 | 352 | 16.913 | 74.475 | 31.430 | 1.00 | 0.00 |
| ATOM | 927 | O | CYS | 2 | 352 | 16.948 | 73.438 | 32.106 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 928 | CB | CYS | 2 | 352 | 14.744 | 75.453 | 32.082 | 1.00 | 0.00 |
| ATOM | 929 | SG | CYS | 2 | 352 | 14.221 | 74.137 | 33.230 | 1.00 | 0.00 |
| ATOM | 930 | H | CYS | 2 | 352 | 15.619 | 73.353 | 29.477 | 1.00 | 0.00 |
| ATOM | 931 | N | ASP | 2 | 353 | 17.949 | 75.224 | 31.058 | 1.00 | 0.00 |
| ATOM | 932 | CA | ASP | 2 | 353 | 19.333 | 74.834 | 31.282 | 1.00 | 0.00 |
| ATOM | 933 | C | ASP | 2 | 353 | 19.736 | 74.659 | 32.730 | 1.00 | 0.00 |
| ATOM | 934 | O | ASP | 2 | 353 | 19.058 | 75.057 | 33.684 | 1.00 | 0.00 |
| ATOM | 935 | CB | ASP | 2 | 353 | 20.292 | 75.778 | 30.537 | 1.00 | 0.00 |
| ATOM | 936 | CG | ASP | 2 | 353 | 20.220 | 77.195 | 31.080 | 1.00 | 0.00 |
| ATOM | 937 | OD1 | ASP | 2 | 353 | 20.906 | 77.501 | 32.049 | 1.00 | 0.00 |
| ATOM | 938 | OD2 | ASP | 2 | 353 | 19.480 | 78.003 | 30.534 | 1.00 | 0.00 |
| ATOM | 939 | H | ASP | 2 | 353 | 17.811 | 76.119 | 30.637 | 1.00 | 0.00 |
| ATOM | 940 | N | THR | 2 | 354 | 20.800 | 73.967 | 32.817 | 1.00 | 0.00 |
| ATOM | 941 | CA | THR | 2 | 354 | 21.189 | 73.282 | 34.069 | 1.00 | 0.00 |
| ATOM | 942 | C | THR | 2 | 354 | 22.645 | 72.859 | 34.236 | 1.00 | 0.00 |
| ATOM | 943 | O | THR | 2 | 354 | 23.006 | 71.851 | 34.855 | 1.00 | 0.00 |
| ATOM | 944 | CB | THR | 2 | 354 | 20.230 | 72.103 | 34.180 | 1.00 | 0.00 |
| ATOM | 945 | OG1 | THR | 2 | 354 | 20.207 | 71.591 | 35.510 | 1.00 | 0.00 |
| ATOM | 946 | CG2 | THR | 2 | 354 | 20.523 | 71.010 | 33.144 | 1.00 | 0.00 |
| ATOM | 947 | H | THR | 2 | 354 | 21.284 | 73.685 | 31.944 | 1.00 | 0.00 |
| ATOM | 948 | HG1 | THR | 2 | 354 | 20.418 | 72.354 | 36.052 | 1.00 | 0.00 |
| ATOM | 949 | N | MET | 2 | 355 | 23.491 | 73.675 | 33.592 | 1.00 | 0.00 |
| ATOM | 950 | CA | MET | 2 | 355 | 24.881 | 73.303 | 33.819 | 1.00 | 0.00 |
| ATOM | 951 | C | MET | 2 | 355 | 25.407 | 74.086 | 34.998 | 1.00 | 0.00 |
| ATOM | 952 | O | MET | 2 | 355 | 24.958 | 75.204 | 35.264 | 1.00 | 0.00 |
| ATOM | 953 | CB | MET | 2 | 355 | 25.714 | 73.520 | 32.553 | 1.00 | 0.00 |
| ATOM | 954 | CG | MET | 2 | 355 | 26.975 | 72.651 | 32.519 | 1.00 | 0.00 |
| ATOM | 955 | SD | MET | 2 | 355 | 27.945 | 72.883 | 31.023 | 1.00 | 0.00 |
| ATOM | 956 | CE | MET | 2 | 355 | 29.154 | 71.577 | 31.307 | 1.00 | 0.00 |
| ATOM | 957 | H | MET | 2 | 355 | 23.207 | 74.584 | 33.288 | 1.00 | 0.00 |
| ATOM | 958 | N | LYS | 2 | 356 | 26.374 | 73.491 | 35.688 | 1.00 | 0.00 |
| ATOM | 959 | CA | LYS | 2 | 356 | 27.020 | 74.312 | 36.693 | 1.00 | 0.00 |
| ATOM | 960 | C | LYS | 2 | 356 | 28.517 | 74.153 | 36.649 | 1.00 | 0.00 |
| ATOM | 961 | O | LYS | 2 | 356 | 29.118 | 73.483 | 37.492 | 1.00 | 0.00 |
| ATOM | 962 | CB | LYS | 2 | 356 | 26.408 | 74.019 | 38.058 | 1.00 | 0.00 |
| ATOM | 963 | CG | LYS | 2 | 356 | 26.879 | 75.024 | 39.094 | 1.00 | 0.00 |
| ATOM | 964 | CD | LYS | 2 | 356 | 26.664 | 76.484 | 38.707 | 1.00 | 0.00 |
| ATOM | 965 | CE | LYS | 2 | 356 | 27.129 | 77.395 | 39.837 | 1.00 | 0.00 |
| ATOM | 966 | NZ | LYS | 2 | 356 | 26.237 | 77.232 | 40.980 | 1.00 | 0.00 |
| ATOM | 967 | H | LYS | 2 | 356 | 26.659 | 72.578 | 35.404 | 1.00 | 0.00 |
| ATOM | 968 | 1HZ | LYS | 2 | 356 | 25.306 | 77.669 | 40.853 | 1.00 | 0.00 |
| ATOM | 969 | 2HZ | LYS | 2 | 356 | 26.029 | 76.234 | 41.150 | 1.00 | 0.00 |
| ATOM | 970 | 3HZ | LYS | 2 | 356 | 26.627 | 77.631 | 41.845 | 1.00 | 0.00 |
| ATOM | 971 | N | VAL | 2 | 357 | 29.079 | 74.753 | 35.579 | 1.00 | 0.00 |
| ATOM | 972 | CA | VAL | 2 | 357 | 30.483 | 74.591 | 35.174 | 1.00 | 0.00 |
| ATOM | 973 | C | VAL | 2 | 357 | 30.833 | 73.208 | 34.631 | 1.00 | 0.00 |
| ATOM | 974 | O | VAL | 2 | 357 | 31.347 | 73.049 | 33.521 | 1.00 | 0.00 |
| ATOM | 975 | CB | VAL | 2 | 357 | 31.465 | 75.058 | 36.271 | 1.00 | 0.00 |
| ATOM | 976 | CG1 | VAL | 2 | 357 | 32.932 | 74.942 | 35.841 | 1.00 | 0.00 |
| ATOM | 977 | CG2 | VAL | 2 | 357 | 31.139 | 76.489 | 36.712 | 1.00 | 0.00 |
| ATOM | 978 | H | VAL | 2 | 357 | 28.513 | 75.428 | 35.114 | 1.00 | 0.00 |
| ATOM | 979 | N | GLY | 2 | 358 | 30.501 | 72.187 | 35.435 | 1.00 | 0.00 |
| ATOM | 980 | CA | GLY | 2 | 358 | 30.882 | 70.821 | 35.090 | 1.00 | 0.00 |
| ATOM | 981 | C | GLY | 2 | 358 | 31.940 | 70.290 | 36.040 | 1.00 | 0.00 |
| ATOM | 982 | O | GLY | 2 | 358 | 32.103 | 70.804 | 37.150 | 1.00 | 0.00 |
| ATOM | 983 | H | GLY | 2 | 358 | 30.076 | 72.384 | 36.317 | 1.00 | 0.00 |
| ATOM | 984 | N | GLY | 2 | 359 | 32.632 | 69.250 | 35.523 | 1.00 | 0.00 |
| ATOM | 985 | CA | GLY | 2 | 359 | 33.779 | 68.606 | 36.170 | 1.00 | 0.00 |
| ATOM | 986 | C | GLY | 2 | 359 | 34.259 | 67.462 | 35.280 | 1.00 | 0.00 |
| ATOM | 987 | O | GLY | 2 | 359 | 33.790 | 67.312 | 34.152 | 1.00 | 0.00 |
| ATOM | 988 | H | GLY | 2 | 359 | 32.497 | 68.953 | 34.576 | 1.00 | 0.00 |
| ATOM | 989 | N | ASN | 2 | 360 | 35.186 | 66.635 | 35.793 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 990 | CA | ASN | 2 | 360 | 35.576 | 65.428 | 35.043 | 1.00 | 0.00 |
| ATOM | 991 | C | ASN | 2 | 360 | 35.039 | 64.158 | 35.689 | 1.00 | 0.00 |
| ATOM | 992 | O | ASN | 2 | 360 | 34.506 | 64.230 | 36.810 | 1.00 | 0.00 |
| ATOM | 993 | CB | ASN | 2 | 360 | 37.103 | 65.347 | 34.859 | 1.00 | 0.00 |
| ATOM | 994 | CG | ASN | 2 | 360 | 37.802 | 64.889 | 36.131 | 1.00 | 0.00 |
| ATOM | 995 | OD1 | ASN | 2 | 360 | 37.407 | 65.197 | 37.257 | 1.00 | 0.00 |
| ATOM | 996 | ND2 | ASN | 2 | 360 | 38.859 | 64.105 | 35.925 | 1.00 | 0.00 |
| ATOM | 997 | H | ASN | 2 | 360 | 35.481 | 66.767 | 36.738 | 1.00 | 0.00 |
| ATOM | 998 | 1HD2 | ASN | 2 | 360 | 39.386 | 63.691 | 36.664 | 1.00 | 0.00 |
| ATOM | 999 | 2HD2 | ASN | 2 | 360 | 39.142 | 63.902 | 34.987 | 1.00 | 0.00 |
| ATOM | 1000 | N | LEU | 2 | 361 | 35.237 | 63.018 | 34.967 | 1.00 | 0.00 |
| ATOM | 1001 | CA | LEU | 2 | 361 | 34.876 | 61.684 | 35.470 | 1.00 | 0.00 |
| ATOM | 1002 | C | LEU | 2 | 361 | 35.619 | 60.507 | 34.808 | 1.00 | 0.00 |
| ATOM | 1003 | O | LEU | 2 | 361 | 36.085 | 60.551 | 33.667 | 1.00 | 0.00 |
| ATOM | 1004 | CB | LEU | 2 | 361 | 33.361 | 61.455 | 35.376 | 1.00 | 0.00 |
| ATOM | 1005 | CG | LEU | 2 | 361 | 32.781 | 60.670 | 36.558 | 1.00 | 0.00 |
| ATOM | 1006 | CD1 | LEU | 2 | 361 | 32.729 | 61.510 | 37.835 | 1.00 | 0.00 |
| ATOM | 1007 | CD2 | LEU | 2 | 361 | 31.426 | 60.047 | 36.231 | 1.00 | 0.00 |
| ATOM | 1008 | H | LEU | 2 | 361 | 35.529 | 63.093 | 34.018 | 1.00 | 0.00 |
| ATOM | 1009 | N | ASP | 2 | 362 | 35.672 | 59.417 | 35.601 | 1.00 | 0.00 |
| ATOM | 1010 | CA | ASP | 2 | 362 | 36.262 | 58.113 | 35.261 | 1.00 | 0.00 |
| ATOM | 1011 | C | ASP | 2 | 362 | 36.069 | 57.507 | 33.875 | 1.00 | 0.00 |
| ATOM | 1012 | O | ASP | 2 | 362 | 36.978 | 56.859 | 33.336 | 1.00 | 0.00 |
| ATOM | 1013 | CB | ASP | 2 | 362 | 35.891 | 57.076 | 36.345 | 1.00 | 0.00 |
| ATOM | 1014 | CG | ASP | 2 | 362 | 34.418 | 56.659 | 36.328 | 1.00 | 0.00 |
| ATOM | 1015 | OD1 | ASP | 2 | 362 | 33.562 | 57.453 | 35.953 | 1.00 | 0.00 |
| ATOM | 1016 | OD2 | ASP | 2 | 362 | 34.118 | 55.522 | 36.691 | 1.00 | 0.00 |
| ATOM | 1017 | H | ASP | 2 | 362 | 35.335 | 59.533 | 36.532 | 1.00 | 0.00 |
| ATOM | 1018 | N | SER | 2 | 363 | 34.856 | 57.716 | 33.320 | 1.00 | 0.00 |
| ATOM | 1019 | CA | SER | 2 | 363 | 34.778 | 57.097 | 32.003 | 1.00 | 0.00 |
| ATOM | 1020 | C | SER | 2 | 363 | 35.187 | 57.936 | 30.813 | 1.00 | 0.00 |
| ATOM | 1021 | O | SER | 2 | 363 | 36.340 | 57.849 | 30.390 | 1.00 | 0.00 |
| ATOM | 1022 | CB | SER | 2 | 363 | 33.498 | 56.273 | 31.794 | 1.00 | 0.00 |
| ATOM | 1023 | OG | SER | 2 | 363 | 33.321 | 55.404 | 32.927 | 1.00 | 0.00 |
| ATOM | 1024 | H | SER | 2 | 363 | 34.133 | 58.210 | 33.808 | 1.00 | 0.00 |
| ATOM | 1025 | HG | SER | 2 | 363 | 34.237 | 55.254 | 33.212 | 1.00 | 0.00 |
| ATOM | 1026 | N | LYS | 2 | 364 | 34.221 | 58.658 | 30.234 | 1.00 | 0.00 |
| ATOM | 1027 | CA | LYS | 2 | 364 | 34.404 | 58.693 | 28.792 | 1.00 | 0.00 |
| ATOM | 1028 | C | LYS | 2 | 364 | 35.164 | 59.874 | 28.230 | 1.00 | 0.00 |
| ATOM | 1029 | O | LYS | 2 | 364 | 34.775 | 61.043 | 28.377 | 1.00 | 0.00 |
| ATOM | 1030 | CB | LYS | 2 | 364 | 33.070 | 58.355 | 28.113 | 1.00 | 0.00 |
| ATOM | 1031 | CG | LYS | 2 | 364 | 31.900 | 59.315 | 28.330 | 1.00 | 0.00 |
| ATOM | 1032 | CD | LYS | 2 | 364 | 31.869 | 60.453 | 27.312 | 1.00 | 0.00 |
| ATOM | 1033 | CE | LYS | 2 | 364 | 31.363 | 61.747 | 27.933 | 1.00 | 0.00 |
| ATOM | 1034 | NZ | LYS | 2 | 364 | 32.281 | 62.149 | 28.999 | 1.00 | 0.00 |
| ATOM | 1035 | H | LYS | 2 | 364 | 33.369 | 58.912 | 30.688 | 1.00 | 0.00 |
| ATOM | 1036 | 1HZ | LYS | 2 | 364 | 33.270 | 62.072 | 28.707 | 1.00 | 0.00 |
| ATOM | 1037 | 2HZ | LYS | 2 | 364 | 32.091 | 63.124 | 29.268 | 1.00 | 0.00 |
| ATOM | 1038 | 3HZ | LYS | 2 | 364 | 32.164 | 61.551 | 29.833 | 1.00 | 0.00 |
| ATOM | 1039 | N | GLY | 2 | 365 | 36.255 | 59.474 | 27.580 | 1.00 | 0.00 |
| ATOM | 1040 | CA | GLY | 2 | 365 | 37.192 | 60.395 | 26.954 | 1.00 | 0.00 |
| ATOM | 1041 | C | GLY | 2 | 365 | 38.170 | 59.630 | 26.080 | 1.00 | 0.00 |
| ATOM | 1042 | O | GLY | 2 | 365 | 38.644 | 60.086 | 25.038 | 1.00 | 0.00 |
| ATOM | 1043 | H | GLY | 2 | 365 | 36.349 | 58.486 | 27.486 | 1.00 | 0.00 |
| ATOM | 1044 | N | TYR | 2 | 366 | 38.468 | 58.411 | 26.552 | 1.00 | 0.00 |
| ATOM | 1045 | CA | TYR | 2 | 366 | 38.976 | 57.459 | 25.568 | 1.00 | 0.00 |
| ATOM | 1046 | C | TYR | 2 | 366 | 37.746 | 56.966 | 24.795 | 1.00 | 0.00 |
| ATOM | 1047 | O | TYR | 2 | 366 | 36.614 | 57.179 | 25.246 | 1.00 | 0.00 |
| ATOM | 1048 | CB | TYR | 2 | 366 | 39.816 | 56.369 | 26.273 | 1.00 | 0.00 |
| ATOM | 1049 | CG | TYR | 2 | 366 | 41.059 | 56.889 | 27.010 | 1.00 | 0.00 |
| ATOM | 1050 | CD1 | TYR | 2 | 366 | 41.573 | 58.189 | 26.793 | 1.00 | 0.00 |
| ATOM | 1051 | CD2 | TYR | 2 | 366 | 41.706 | 56.015 | 27.913 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1052 | CE1 | TYR | 2 | 366 | 42.754 | 58.596 | 27.445 | 1.00 | 0.00 |
| ATOM | 1053 | CE2 | TYR | 2 | 366 | 42.890 | 56.415 | 28.565 | 1.00 | 0.00 |
| ATOM | 1054 | CZ | TYR | 2 | 366 | 43.418 | 57.700 | 28.312 | 1.00 | 0.00 |
| ATOM | 1055 | OH | TYR | 2 | 366 | 44.608 | 58.103 | 28.907 | 1.00 | 0.00 |
| ATOM | 1056 | H | TYR | 2 | 366 | 38.101 | 58.130 | 27.436 | 1.00 | 0.00 |
| ATOM | 1057 | HH | TYR | 2 | 366 | 45.136 | 57.300 | 29.048 | 1.00 | 0.00 |
| ATOM | 1058 | N | GLY | 2 | 367 | 37.953 | 56.420 | 23.601 | 1.00 | 0.00 |
| ATOM | 1059 | CA | GLY | 2 | 367 | 36.799 | 56.335 | 22.699 | 1.00 | 0.00 |
| ATOM | 1060 | C | GLY | 2 | 367 | 36.986 | 55.338 | 21.585 | 1.00 | 0.00 |
| ATOM | 1061 | O | GLY | 2 | 367 | 36.066 | 54.684 | 21.071 | 1.00 | 0.00 |
| ATOM | 1062 | H | GLY | 2 | 367 | 38.871 | 56.134 | 23.345 | 1.00 | 0.00 |
| ATOM | 1063 | N | VAL | 2 | 368 | 38.276 | 55.233 | 21.223 | 1.00 | 0.00 |
| ATOM | 1064 | CA | VAL | 2 | 368 | 38.628 | 53.981 | 20.573 | 1.00 | 0.00 |
| ATOM | 1065 | C | VAL | 2 | 368 | 39.403 | 53.086 | 21.533 | 1.00 | 0.00 |
| ATOM | 1066 | O | VAL | 2 | 368 | 40.067 | 53.580 | 22.453 | 1.00 | 0.00 |
| ATOM | 1067 | CB | VAL | 2 | 368 | 39.370 | 54.252 | 19.257 | 1.00 | 0.00 |
| ATOM | 1068 | CG1 | VAL | 2 | 368 | 39.422 | 53.013 | 18.359 | 1.00 | 0.00 |
| ATOM | 1069 | CG2 | VAL | 2 | 368 | 38.720 | 55.418 | 18.506 | 1.00 | 0.00 |
| ATOM | 1070 | H | VAL | 2 | 368 | 38.954 | 55.879 | 21.570 | 1.00 | 0.00 |
| ATOM | 1071 | N | ALA | 2 | 369 | 38.292 | 51.757 | 21.301 | 1.00 | 0.00 |
| ATOM | 1072 | CA | ALA | 2 | 369 | 40.103 | 50.755 | 21.991 | 1.00 | 0.00 |
| ATOM | 1073 | C | ALA | 2 | 369 | 40.986 | 50.017 | 21.008 | 1.00 | 0.00 |
| ATOM | 1074 | O | ALA | 2 | 369 | 40.746 | 50.087 | 19.796 | 1.00 | 0.00 |
| ATOM | 1075 | CB | ALA | 2 | 369 | 39.210 | 49.721 | 22.673 | 1.00 | 0.00 |
| ATOM | 1076 | H | ALA | 2 | 369 | 38.622 | 51.435 | 20.636 | 1.00 | 0.00 |
| ATOM | 1077 | N | THR | 2 | 370 | 41.995 | 49.356 | 21.580 | 1.00 | 0.00 |
| ATOM | 1078 | CA | THR | 2 | 370 | 42.946 | 48.522 | 20.851 | 1.00 | 0.00 |
| ATOM | 1079 | C | THR | 2 | 370 | 43.819 | 47.618 | 21.751 | 1.00 | 0.00 |
| ATOM | 1080 | O | THR | 2 | 370 | 45.033 | 47.567 | 21.570 | 1.00 | 0.00 |
| ATOM | 1081 | CB | THR | 2 | 370 | 43.793 | 49.468 | 19.964 | 1.00 | 0.00 |
| ATOM | 1082 | OG1 | THR | 2 | 370 | 44.807 | 48.770 | 19.218 | 1.00 | 0.00 |
| ATOM | 1083 | CG2 | THR | 2 | 370 | 44.407 | 50.614 | 20.777 | 1.00 | 0.00 |
| ATOM | 1084 | H | THR | 2 | 370 | 42.019 | 49.382 | 22.576 | 1.00 | 0.00 |
| ATOM | 1085 | HG1 | THR | 2 | 370 | 45.365 | 483461 | 19.944 | 1.00 | 0.00 |
| ATOM | 1086 | N | PRO | 2 | 371 | 43.216 | 46.903 | 22.745 | 1.00 | 0.00 |
| ATOM | 1087 | CA | PRO | 2 | 371 | 44.010 | 46.190 | 23.735 | 1.00 | 0.00 |
| ATOM | 1088 | C | PRO | 2 | 371 | 45.129 | 45.274 | 23.215 | 1.00 | 0.00 |
| ATOM | 1089 | O | PRO | 2 | 371 | 44.890 | 44.314 | 22.467 | 1.00 | 0.00 |
| ATOM | 1090 | CB | PRO | 2 | 371 | 43.024 | 45.448 | 24.597 | 1.00 | 0.00 |
| ATOM | 1091 | CG | PRO | 2 | 371 | 41.759 | 46.283 | 24.474 | 1.00 | 0.00 |
| ATOM | 1092 | CD | PRO | 2 | 371 | 41.796 | 46.769 | 23.048 | 1.00 | 0.00 |
| ATOM | 1093 | N | LYS | 2 | 372 | 46.346 | 45.646 | 23.662 | 1.00 | 0.00 |
| ATOM | 1094 | CA | LYS | 2 | 372 | 47.537 | 44.799 | 23.677 | 1.00 | 0.00 |
| ATOM | 1095 | C | LYS | 2 | 372 | 47.823 | 44.047 | 22.394 | 1.00 | 0.00 |
| ATOM | 1096 | O | LYS | 2 | 372 | 48.641 | 44.435 | 21.560 | 1.00 | 0.00 |
| ATOM | 1097 | CB | LYS | 2 | 372 | 47.491 | 43.853 | 24.891 | 1.00 | 0.00 |
| ATOM | 1098 | CG | LYS | 2 | 372 | 48.353 | 44.204 | 26.117 | 1.00 | 0.00 |
| ATOM | 1099 | CD | LYS | 2 | 372 | 48.053 | 45.548 | 26.786 | 1.00 | 0.00 |
| ATOM | 1100 | CE | LYS | 2 | 372 | 49.931 | 46.685 | 26.260 | 1.00 | 0.00 |
| ATOM | 1101 | NZ | LYS | 2 | 372 | 48.513 | 47.943 | 26.871 | 1.00 | 0.00 |
| ATOM | 1102 | H | LYS | 2 | 372 | 46.404 | 46.554 | 24.085 | 1.00 | 0.00 |
| ATOM | 1103 | 1HZ | LYS | 2 | 372 | 48.205 | 47.775 | 27.841 | 1.00 | 0.00 |
| ATOM | 1104 | 2HZ | LYS | 2 | 372 | 49.328 | 48.571 | 26.986 | 1.00 | 0.00 |
| ATOM | 1105 | 3HZ | LYS | 2 | 372 | 47.743 | 48.402 | 26.341 | 1.00 | 0.00 |
| ATOM | 1106 | N | GLY | 2 | 373 | 47.090 | 42.934 | 22.246 | 1.00 | 0.00 |
| ATOM | 1107 | CA | GLY | 2 | 373 | 47.313 | 42.011 | 21.135 | 1.00 | 0.00 |
| ATOM | 1108 | C | GLY | 2 | 373 | 47.226 | 42.547 | 19.706 | 1.00 | 0.00 |
| ATOM | 1109 | O | GLY | 2 | 373 | 47.436 | 41.796 | 18.753 | 1.00 | 0.00 |
| ATOM | 1110 | H | GLY | 2 | 373 | 46.367 | 42.795 | 22.924 | 1.00 | 0.00 |
| ATOM | 1111 | N | SER | 2 | 374 | 46.926 | 43.846 | 19.545 | 1.00 | 0.00 |
| ATOM | 1112 | CA | SER | 2 | 374 | 47.157 | 44.442 | 18.232 | 1.00 | 0.00 |
| ATOM | 1113 | C | SER | 2 | 374 | 47.540 | 45.903 | 18.279 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1114 | O | SER | 2 | 374 | 47.007 | 46.713 | 19.033 | 1.00 | 0.00 |
| ATOM | 1115 | CB | SER | 2 | 374 | 45.944 | 44.288 | 17.329 | 1.00 | 0.00 |
| ATOM | 1116 | OG | SER | 2 | 374 | 45.792 | 42.917 | 16.941 | 1.00 | 0.00 |
| ATOM | 1117 | H | SER | 2 | 374 | 46.725 | 44.454 | 20.316 | 1.00 | 0.00 |
| ATOM | 1118 | HG | SER | 2 | 374 | 45.932 | 42.385 | 17.724 | 1.00 | 0.00 |
| ATOM | 1119 | N | ALA | 2 | 375 | 48.486 | 46.238 | 17.388 | 1.00 | 0.00 |
| ATOM | 1120 | CA | ALA | 2 | 375 | 48.902 | 47.636 | 17.257 | 1.00 | 0.00 |
| ATOM | 1121 | C | ALA | 2 | 375 | 47.990 | 48.502 | 16.389 | 1.00 | 0.00 |
| ATOM | 1122 | O | ALA | 2 | 375 | 48.424 | 49.315 | 15.570 | 1.00 | 0.00 |
| ATOM | 1123 | CB | ALA | 2 | 375 | 50.332 | 47.689 | 16.715 | 1.00 | 0.00 |
| ATOM | 1124 | H | ALA | 2 | 375 | 48.890 | 45.518 | 16.830 | 1.00 | 0.00 |
| ATOM | 1125 | N | LEU | 2 | 376 | 46.673 | 48.276 | 16.592 | 1.00 | 0.00 |
| ATOM | 1126 | CA | LEU | 2 | 376 | 45.682 | 49.143 | 15.954 | 1.00 | 0.00 |
| ATOM | 1127 | C | LEU | 2 | 376 | 45.771 | 50.567 | 16.469 | 1.00 | 0.00 |
| ATOM | 1128 | O | LEU | 2 | 376 | 45.368 | 51.515 | 15.805 | 1.00 | 0.00 |
| ATOM | 1129 | CB | LEU | 2 | 376 | 44.249 | 48.658 | 16.193 | 1.00 | 0.00 |
| ATOM | 1130 | CG | LEU | 2 | 376 | 44.024 | 47.148 | 16.150 | 1.00 | 0.00 |
| ATOM | 1131 | CD1 | LEU | 2 | 376 | 42.767 | 46.753 | 16.923 | 1.00 | 0.00 |
| ATOM | 1132 | CD2 | LEU | 2 | 376 | 44.030 | 46.595 | 14.728 | 1.00 | 0.00 |
| ATOM | 1133 | H | LEU | 2 | 376 | 46.456 | 47.762 | 17.420 | 1.00 | 0.00 |
| ATOM | 1134 | N | GLY | 2 | 377 | 46.336 | 50.662 | 17.682 | 1.00 | 0.00 |
| ATOM | 1135 | CA | GLY | 2 | 377 | 46.646 | 51.939 | 18.325 | 1.00 | 0.00 |
| ATOM | 1136 | C | GLY | 2 | 377 | 47.290 | 52.942 | 17.401 | 1.00 | 0.00 |
| ATOM | 1137 | O | GLY | 2 | 377 | 46.819 | 54.061 | 17.224 | 1.00 | 0.00 |
| ATOM | 1138 | H | GLY | 2 | 377 | 46.515 | 49.796 | 18.148 | 1.00 | 0.00 |
| ATOM | 1139 | N | ASN | 2 | 378 | 48.350 | 52.466 | 16.726 | 1.00 | 0.00 |
| ATOM | 1140 | CA | ASN | 2 | 378 | 49.029 | 53.310 | 15.727 | 1.00 | 0.00 |
| ATOM | 1141 | C | ASN | 2 | 378 | 48.098 | 53.943 | 14.694 | 1.00 | 0.00 |
| ATOM | 1142 | O | ASN | 2 | 378 | 48.196 | 55.125 | 14.343 | 1.00 | 0.00 |
| ATOM | 1143 | CB | ASN | 2 | 378 | 50.136 | 52.546 | 14.979 | 1.00 | 0.00 |
| ATOM | 1144 | CG | ASN | 2 | 378 | 51.052 | 51.799 | 15.931 | 1.00 | 0.00 |
| ATOM | 1145 | OD1 | ASN | 2 | 378 | 50.643 | 50.880 | 16.626 | 1.00 | 0.00 |
| ATOM | 1146 | ND2 | ASN | 2 | 378 | 52.321 | 52.210 | 15.947 | 1.00 | 0.00 |
| ATOM | 1147 | H | ASN | 2 | 378 | 48.712 | 51.579 | 17.033 | 1.00 | 0.00 |
| ATOM | 1148 | 1HD2 | ASN | 2 | 378 | 52.968 | 51.789 | 16.588 | 1.00 | 0.00 |
| ATOM | 1149 | 2HD2 | ASN | 2 | 378 | 52.683 | 52.906 | 15.325 | 1.00 | 0.00 |
| ATOM | 1150 | N | ALA | 2 | 379 | 47.174 | 53.076 | 14.232 | 1.00 | 0.00 |
| ATOM | 1151 | CA | ALA | 2 | 379 | 46.218 | 53.594 | 13.261 | 1.00 | 0.00 |
| ATOM | 1152 | C | ALA | 2 | 379 | 45.327 | 54.674 | 13.840 | 1.00 | 0.00 |
| ATOM | 1153 | O | ALA | 2 | 379 | 45.123 | 55.734 | 13.249 | 1.00 | 0.00 |
| ATOM | 1154 | CB | ALA | 2 | 379 | 45.350 | 52.470 | 12.687 | 1.00 | 0.00 |
| ATOM | 1155 | H | ALA | 2 | 379 | 46.992 | 52.239 | 14.750 | 1.00 | 0.00 |
| ATOM | 1156 | N | VAL | 2 | 380 | 44.814 | 54.409 | 15.053 | 1.00 | 0.00 |
| ATOM | 1157 | CA | VAL | 2 | 380 | 43.858 | 55.372 | 15.617 | 1.00 | 0.00 |
| ATOM | 1158 | C | VAL | 2 | 380 | 44.423 | 56.777 | 15.821 | 1.00 | 0.00 |
| ATOM | 1159 | O | VAL | 2 | 380 | 43.834 | 57.806 | 15.484 | 1.00 | 0.00 |
| ATOM | 1160 | CB | VAL | 2 | 380 | 43.245 | 54.945 | 16.914 | 1.00 | 0.00 |
| ATOM | 1161 | CG1 | VAL | 2 | 380 | 42.087 | 55.751 | 17.322 | 1.00 | 0.00 |
| ATOM | 1162 | CG2 | VAL | 2 | 380 | 42.796 | 53.387 | 16.792 | 1.00 | 0.00 |
| ATOM | 1163 | H | VAL | 2 | 380 | 45.044 | 53.551 | 15.513 | 1.00 | 0.00 |
| ATOM | 1164 | N | ASN | 2 | 381 | 45.676 | 56.765 | 16.316 | 1.00 | 0.00 |
| ATOM | 1165 | CA | ASN | 2 | 381 | 46.383 | 58.044 | 16.391 | 1.00 | 0.00 |
| ATOM | 1166 | C | ASN | 2 | 381 | 46.407 | 58.796 | 15.071 | 1.00 | 0.00 |
| ATOM | 1167 | O | ASN | 2 | 381 | 45.797 | 59.847 | 14.955 | 1.00 | 0.00 |
| ATOM | 1168 | CB | ASN | 2 | 381 | 47.794 | 57.895 | 16.968 | 1.00 | 0.00 |
| ATOM | 1169 | CG | ASN | 2 | 381 | 48.367 | 59.281 | 17.221 | 1.00 | 0.00 |
| ATOM | 1170 | OD1 | ASN | 2 | 381 | 49.196 | 59.799 | 16.483 | 1.00 | 0.00 |
| ATOM | 1171 | ND2 | ASN | 2 | 381 | 47.867 | 59.879 | 18.308 | 1.00 | 0.00 |
| ATOM | 1172 | H | ASN | 2 | 381 | 46.070 | 55.952 | 16.751 | 1.00 | 0.00 |
| ATOM | 1173 | 1HD2 | ASN | 2 | 381 | 48.250 | 60.754 | 18.599 | 1.00 | 0.00 |
| ATOM | 1174 | 2HD2 | ASN | 2 | 381 | 47.118 | 59.465 | 18.834 | 1.00 | 0.00 |
| ATOM | 1175 | N | LEU | 2 | 382 | 47.065 | 58.185 | 14.069 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1176 | CA | LEU | 2 | 382 | 47.081 | 58.801 | 12.735 | 1.00 | 0.00 |
| ATOM | 1177 | C | LEU | 2 | 382 | 45.740 | 59.364 | 12.260 | 1.00 | 0.00 |
| ATOM | 1178 | O | LEU | 2 | 382 | 45.618 | 60.470 | 11.750 | 1.00 | 0.00 |
| ATOM | 1179 | CB | LEU | 2 | 382 | 47.643 | 57.799 | 11.721 | 1.00 | 0.00 |
| ATOM | 1180 | CG | LEU | 2 | 382 | 47.891 | 58.375 | 10.322 | 1.00 | 0.00 |
| ATOM | 1181 | CD1 | LEU | 2 | 382 | 48.913 | 59.515 | 10.335 | 1.00 | 0.00 |
| ATOM | 1182 | CD2 | LEU | 2 | 382 | 48.263 | 57.280 | 9.322 | 1.00 | 0.00 |
| ATOM | 1183 | H | LEU | 2 | 382 | 47.617 | 57.375 | 14.265 | 1.00 | 0.00 |
| ATOM | 1184 | N | ALA | 2 | 383 | 44.710 | 58.539 | 12.502 | 1.00 | 0.00 |
| ATOM | 1185 | CA | ALA | 2 | 383 | 43.355 | 58.962 | 12.152 | 1.00 | 0.00 |
| ATOM | 1186 | C | ALA | 2 | 383 | 42.842 | 60.215 | 12.849 | 1.00 | 0.00 |
| ATOM | 1187 | O | ALA | 2 | 383 | 42.851 | 61.300 | 12.276 | 1.00 | 0.00 |
| ATOM | 1188 | CB | ALA | 2 | 383 | 42.367 | 57.806 | 12.338 | 1.00 | 0.00 |
| ATOM | 1189 | H | ALA | 2 | 383 | 44.899 | 57.714 | 13.034 | 1.00 | 0.00 |
| ATOM | 1190 | N | VAL | 2 | 384 | 42.360 | 60.058 | 14.093 | 1.00 | 0.00 |
| ATOM | 1191 | CA | VAL | 2 | 384 | 41.676 | 61.197 | 14.723 | 1.00 | 0.00 |
| ATOM | 1192 | C | VAL | 2 | 384 | 43.608 | 62.303 | 15.228 | 1.00 | 0.00 |
| ATOM | 1193 | O | VAL | 2 | 384 | 42.231 | 63.359 | 15.729 | 1.00 | 0.00 |
| ATOM | 1194 | CB | VAL | 2 | 384 | 40.708 | 60.719 | 15.821 | 1.00 | 0.00 |
| ATOM | 1195 | CG1 | VAL | 2 | 384 | 39.622 | 61.762 | 16.105 | 1.00 | 0.00 |
| ATOM | 1196 | CG2 | VAL | 2 | 384 | 40.064 | 59.374 | 15.475 | 1.00 | 0.00 |
| ATOM | 1197 | H | VAL | 2 | 384 | 42.584 | 59.215 | 14.579 | 1.00 | 0.00 |
| ATOM | 1198 | N | LEU | 2 | 385 | 43.907 | 62.030 | 15.064 | 1.00 | 0.00 |
| ATOM | 1199 | CA | LEU | 2 | 385 | 44.806 | 63.172 | 14.999 | 1.00 | 0.00 |
| ATOM | 1200 | C | LEU | 2 | 385 | 44.788 | 63.857 | 13.642 | 1.00 | 0.00 |
| ATOM | 1201 | O | LEU | 2 | 385 | 44.546 | 65.051 | 13.561 | 1.00 | 0.00 |
| ATOM | 1202 | CB | LEU | 2 | 385 | 46.223 | 62.814 | 15.452 | 1.00 | 0.00 |
| ATOM | 1203 | CG | LEU | 2 | 385 | 47.048 | 64.019 | 15.911 | 1.00 | 0.00 |
| ATOM | 1204 | CD1 | LEU | 2 | 385 | 46.386 | 54.758 | 17.079 | 1.00 | 0.00 |
| ATOM | 1205 | CD2 | LEU | 2 | 385 | 48.485 | 63.614 | 16.238 | 1.00 | 0.00 |
| ATOM | 1206 | H | LEU | 2 | 385 | 44.195 | 61.124 | 14.760 | 1.00 | 0.00 |
| ATOM | 1207 | N | LYS | 2 | 386 | 45.012 | 63.106 | 12.553 | 1.00 | 0.00 |
| ATOM | 1208 | CA | LYS | 2 | 386 | 44.980 | 63.837 | 11.281 | 1.00 | 0.00 |
| ATOM | 1209 | C | LYS | 2 | 386 | 43.587 | 64.054 | 10.677 | 1.00 | 0.00 |
| ATOM | 1210 | O | LYS | 2 | 386 | 43.404 | 64.438 | 9.518 | 1.00 | 0.00 |
| ATOM | 1211 | CB | LYS | 2 | 386 | 46.001 | 63.255 | 10.292 | 1.00 | 0.00 |
| ATOM | 1212 | CG | LYS | 2 | 386 | 46.597 | 64.307 | 9.347 | 1.00 | 0.00 |
| ATOM | 1213 | CD | LYS | 2 | 386 | 46.042 | 64.252 | 7.920 | 1.00 | 0.00 |
| ATOM | 1214 | CE | LYS | 2 | 386 | 45.833 | 65.645 | 7.319 | 1.00 | 0.00 |
| ATOM | 1215 | NZ | LYS | 2 | 386 | 44.704 | 66.302 | 7.985 | 1.00 | 0.00 |
| ATOM | 1216 | H | LYS | 2 | 386 | 44.969 | 62.109 | 12.598 | 1.00 | 0.00 |
| ATOM | 1217 | 1HZ | LYS | 2 | 386 | 44.941 | 67.275 | 8.254 | 1.00 | 0.00 |
| ATOM | 1218 | 2HZ | LYS | 2 | 386 | 43.823 | 66.318 | 7.445 | 1.00 | 0.00 |
| ATOM | 1219 | 3HZ | LYS | 2 | 386 | 44.435 | 65.865 | 8.903 | 1.00 | 0.00 |
| ATOM | 1220 | N | LEU | 2 | 387 | 42.589 | 63.798 | 11.533 | 1.00 | 0.00 |
| ATOM | 1221 | CA | LEU | 2 | 387 | 41.236 | 64.308 | 11.306 | 1.00 | 0.00 |
| ATOM | 1222 | C | LEU | 2 | 387 | 40.900 | 65.419 | 12.295 | 1.00 | 0.00 |
| ATOM | 1223 | O | LEU | 2 | 387 | 39.761 | 65.862 | 12.468 | 1.00 | 0.00 |
| ATOM | 1224 | CB | LEU | 2 | 387 | 40.196 | 63.187 | 11.420 | 1.00 | 0.00 |
| ATOM | 1225 | CG | LEU | 2 | 387 | 40.418 | 61.981 | 10.497 | 1.00 | 0.00 |
| ATOM | 1226 | CD1 | LEU | 2 | 387 | 39.437 | 60.850 | 10.811 | 1.00 | 0.00 |
| ATOM | 1227 | CD2 | LEU | 2 | 387 | 40.419 | 62.349 | 9.013 | 1.00 | 0.00 |
| ATOM | 1228 | H | LEU | 2 | 387 | 42.815 | 63.323 | 12.383 | 1.00 | 0.00 |
| ATOM | 1229 | N | ASN | 2 | 388 | 41.959 | 65.831 | 13.005 | 1.00 | 0.00 |
| ATOM | 1230 | CA | ASN | 2 | 388 | 41.752 | 66.780 | 14.087 | 1.00 | 0.00 |
| ATOM | 1231 | C | ASN | 2 | 388 | 42.241 | 68.159 | 13.771 | 1.00 | 0.00 |
| ATOM | 1232 | O | ASN | 2 | 388 | 41.510 | 69.116 | 14.001 | 1.00 | 0.00 |
| ATOM | 1233 | CB | ASN | 2 | 388 | 42.358 | 66.337 | 15.415 | 1.00 | 0.00 |
| ATOM | 1234 | CG | ASN | 2 | 388 | 41.231 | 66.181 | 16.407 | 1.00 | 0.00 |
| ATOM | 1235 | OD1 | ASN | 2 | 388 | 40.123 | 65.775 | 16.055 | 1.00 | 0.00 |
| ATOM | 1236 | ND2 | ASN | 2 | 388 | 41.525 | 66.605 | 17.638 | 1.00 | 0.00 |
| ATOM | 1237 | H | ASN | 2 | 388 | 42.894 | 65.593 | 12.742 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1238 | 1HD2 | ASN | 2 | 388 | 40.777 | 66.689 | 18.300 | 1.00 | 0.00 |
| ATOM | 1239 | 2HD2 | ASN | 2 | 388 | 42.475 | 66.811 | 17.886 | 1.00 | 0.00 |
| ATOM | 1240 | N | GLU | 2 | 389 | 43.458 | 68.208 | 13.225 | 1.00 | 0.00 |
| ATOM | 1241 | CA | GLU | 2 | 389 | 43.967 | 69.493 | 12.734 | 1.00 | 0.00 |
| ATOM | 1242 | C | GLU | 2 | 389 | 43.166 | 70.080 | 11.580 | 1.00 | 0.00 |
| ATOM | 1243 | O | GLU | 2 | 389 | 43.157 | 71.273 | 11.305 | 1.00 | 0.00 |
| ATOM | 1244 | CB | GLU | 2 | 389 | 45.459 | 69.405 | 12.368 | 1.00 | 0.00 |
| ATOM | 1245 | CG | GLU | 2 | 389 | 45.935 | 68.154 | 11.607 | 1.00 | 0.00 |
| ATOM | 1246 | CD | GLU | 2 | 389 | 45.076 | 67.881 | 10.387 | 1.00 | 0.00 |
| ATOM | 1247 | OE1 | GLU | 2 | 389 | 44.279 | 66.959 | 10.414 | 1.00 | 0.00 |
| ATOM | 1248 | OE2 | GLU | 2 | 389 | 45.165 | 68.579 | 9.389 | 1.00 | 0.00 |
| ATOM | 1249 | H | GLU | 2 | 389 | 43.945 | 67.352 | 13.033 | 1.00 | 0.00 |
| ATOM | 1250 | N | GLN | 2 | 390 | 42.447 | 69.183 | 10.886 | 1.00 | 0.00 |
| ATOM | 1251 | CA | GLN | 2 | 390 | 41.512 | 69.667 | 9.866 | 1.00 | 0.00 |
| ATOM | 1252 | C | GLN | 2 | 390 | 40.128 | 70.010 | 10.406 | 1.00 | 0.00 |
| ATOM | 1253 | O | GLN | 2 | 390 | 39.182 | 70.368 | 9.701 | 1.00 | 0.00 |
| ATOM | 1254 | CB | GLN | 2 | 390 | 41.440 | 68.655 | 8.722 | 1.00 | 0.00 |
| ATOM | 1255 | CG | GLN | 2 | 390 | 41.015 | 67.260 | 9.182 | 1.00 | 0.00 |
| ATOM | 1256 | CD | GLN | 2 | 390 | 41.130 | 66.296 | 8.026 | 1.00 | 0.00 |
| ATOM | 1257 | OE1 | GLN | 2 | 390 | 42.123 | 66.225 | 7.308 | 1.00 | 0.00 |
| ATOM | 1258 | NE2 | GLN | 2 | 390 | 40.034 | 65.569 | 7.804 | 1.00 | 0.00 |
| ATOM | 1259 | H | GLN | 2 | 390 | 42.650 | 68.217 | 11.056 | 1.00 | 0.00 |
| ATOM | 1260 | 1HE2 | GLN | 2 | 390 | 39.946 | 65.009 | 6.985 | 1.00 | 0.00 |
| ATOM | 1261 | 2HE2 | GLN | 2 | 390 | 39.304 | 65.608 | 8.485 | 1.00 | 0.00 |
| ATOM | 1262 | N | GLY | 2 | 391 | 40.030 | 69.839 | 11.740 | 1.00 | 0.00 |
| ATOM | 1263 | CA | GLY | 2 | 391 | 38.755 | 70.051 | 12.418 | 1.00 | 0.00 |
| ATOM | 1264 | C | GLY | 2 | 391 | 37.623 | 69.133 | 11.997 | 1.00 | 0.00 |
| ATOM | 1265 | O | GLY | 2 | 391 | 36.449 | 69.488 | 12.157 | 1.00 | 0.00 |
| ATOM | 1266 | H | GLY | 2 | 391 | 40.074 | 69.699 | 12.260 | 1.00 | 0.00 |
| ATOM | 1267 | N | LEU | 2 | 392 | 38.006 | 67.950 | 11.479 | 1.00 | 0.00 |
| ATOM | 1268 | CA | LEU | 2 | 392 | 36.907 | 67.054 | 11.140 | 1.00 | 0.00 |
| ATOM | 1269 | C | LEU | 2 | 392 | 36.081 | 66.698 | 12.359 | 1.00 | 0.00 |
| ATOM | 1270 | O | LEU | 2 | 392 | 34.859 | 66.699 | 12.314 | 1.00 | 0.00 |
| ATOM | 1271 | CB | LEU | 2 | 392 | 37.392 | 65.801 | 10.407 | 1.00 | 0.00 |
| ATOM | 1272 | CG | LEU | 2 | 392 | 36.268 | 65.013 | 9.728 | 1.00 | 0.00 |
| ATOM | 1273 | CD1 | LEU | 2 | 392 | 35.659 | 65.789 | 8.559 | 1.00 | 0.00 |
| ATOM | 1274 | CD2 | LEU | 2 | 392 | 36.715 | 63.614 | 9.305 | 1.00 | 0.00 |
| ATOM | 1275 | H | LEU | 2 | 392 | 38.952 | 67.656 | 11.581 | 1.00 | 0.00 |
| ATOM | 1276 | N | LEU | 2 | 393 | 36.805 | 66.473 | 13.474 | 1.00 | 0.00 |
| ATOM | 1277 | CA | LEU | 2 | 393 | 36.123 | 66.183 | 14.742 | 1.00 | 0.00 |
| ATOM | 1278 | C | LEU | 2 | 393 | 35.016 | 67.149 | 15.135 | 1.00 | 0.00 |
| ATOM | 1279 | O | LEU | 2 | 393 | 33.870 | 66.755 | 15.288 | 1.00 | 0.00 |
| ATOM | 1280 | CB | LEU | 2 | 393 | 37.126 | 66.041 | 15.881 | 1.00 | 0.00 |
| ATOM | 1281 | CG | LEU | 2 | 393 | 36.631 | 65.166 | 17.034 | 1.00 | 0.00 |
| ATOM | 1282 | CD1 | LEU | 2 | 393 | 36.308 | 63.750 | 16.559 | 1.00 | 0.00 |
| ATOM | 1283 | CD2 | LEU | 2 | 393 | 37.619 | 65.150 | 18.200 | 1.00 | 0.00 |
| ATOM | 1284 | H | LEU | 2 | 393 | 37.801 | 66.445 | 13.352 | 1.00 | 0.00 |
| ATOM | 1285 | N | ASP | 2 | 394 | 35.362 | 68.460 | 15.207 | 1.00 | 0.00 |
| ATOM | 1286 | CA | ASP | 2 | 394 | 34.270 | 69.421 | 15.492 | 1.00 | 0.00 |
| ATOM | 1287 | C | ASP | 2 | 394 | 33.103 | 69.311 | 14.518 | 1.00 | 0.00 |
| ATOM | 1288 | O | ASP | 2 | 394 | 31.941 | 69.076 | 14.853 | 1.00 | 0.00 |
| ATOM | 1289 | CB | ASP | 2 | 394 | 34.747 | 70.886 | 15.613 | 1.00 | 0.00 |
| ATOM | 1290 | CG | ASP | 2 | 394 | 33.606 | 71.825 | 16.035 | 1.00 | 0.00 |
| ATOM | 1291 | OD1 | ASP | 2 | 394 | 33.183 | 72.653 | 15.232 | 1.00 | 0.00 |
| ATOM | 1292 | OD2 | ASP | 2 | 394 | 33.122 | 71.733 | 17.163 | 1.00 | 0.00 |
| ATOM | 1293 | H | ASP | 2 | 394 | 36.319 | 68.744 | 15.153 | 1.00 | 0.00 |
| ATOM | 1294 | N | LYS | 2 | 395 | 33.485 | 69.360 | 13.242 | 1.00 | 0.00 |
| ATOM | 1295 | CA | LYS | 2 | 395 | 32.507 | 69.101 | 12.184 | 1.00 | 0.00 |
| ATOM | 1296 | C | LYS | 2 | 395 | 31.657 | 67.837 | 12.377 | 1.00 | 0.00 |
| ATOM | 1297 | O | LYS | 2 | 395 | 30.491 | 67.728 | 12.008 | 1.00 | 0.00 |
| ATOM | 1298 | CB | LYS | 2 | 395 | 33.292 | 69.073 | 10.889 | 1.00 | 0.00 |
| ATOM | 1299 | CG | LYS | 2 | 395 | 32.504 | 69.158 | 9.598 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1300 | CD | LYS | 2 | 395 | 33.543 | 69.028 | 8.502 | 1.00 | 0.00 |
| ATOM | 1301 | CE | LYS | 2 | 395 | 32.998 | 69.174 | 7.097 | 1.00 | 0.00 |
| ATOM | 1302 | NZ | LYS | 2 | 395 | 34.120 | 68.873 | 6.205 | 1.00 | 0.00 |
| ATOM | 1303 | H | LYS | 2 | 395 | 34.432 | 69.624 | 13.072 | 1.00 | 0.00 |
| ATOM | 1304 | 1HZ | LYS | 2 | 395 | 34.357 | 67.864 | 6.266 | 1.00 | 0.00 |
| ATOM | 1305 | 2HZ | LYS | 2 | 395 | 33.856 | 69.126 | 5.236 | 1.00 | 0.00 |
| ATOM | 1306 | 3HZ | LYS | 2 | 395 | 34.948 | 69.427 | 6.503 | 1.00 | 0.00 |
| ATOM | 1307 | N | LEU | 2 | 396 | 32.272 | 66.867 | 13.052 | 1.00 | 0.00 |
| ATOM | 1308 | CA | LEU | 2 | 396 | 31.581 | 65.615 | 13.333 | 1.00 | 0.00 |
| ATOM | 1309 | C | LEU | 2 | 396 | 30.696 | 65.582 | 14.573 | 1.00 | 0.00 |
| ATOM | 1310 | O | LEU | 2 | 396 | 29.575 | 65.093 | 14.489 | 1.00 | 0.00 |
| ATOM | 1311 | CB | LEU | 2 | 396 | 32.567 | 64.444 | 13.294 | 1.00 | 0.00 |
| ATOM | 1312 | CG | LEU | 2 | 396 | 32.429 | 63.574 | 12.039 | 1.00 | 0.00 |
| ATOM | 1313 | CD1 | LEU | 2 | 396 | 32.507 | 64.374 | 10.737 | 1.00 | 0.00 |
| ATOM | 1314 | CD2 | LEU | 2 | 396 | 33.425 | 62.417 | 12.048 | 1.00 | 0.00 |
| ATOM | 1315 | H | LEU | 2 | 396 | 33.219 | 66.979 | 13.353 | 1.00 | 0.00 |
| ATOM | 1316 | N | LYS | 2 | 397 | 31.202 | 66.115 | 15.705 | 1.00 | 0.00 |
| ATOM | 1317 | CA | LYS | 2 | 397 | 30.365 | 66.234 | 16.914 | 1.00 | 0.00 |
| ATOM | 1318 | C | LYS | 2 | 397 | 29.303 | 67.315 | 16.888 | 1.00 | 0.00 |
| ATOM | 1319 | O | LYS | 2 | 397 | 28.351 | 67.326 | 17.675 | 1.00 | 0.00 |
| ATOM | 1320 | CB | LYS | 2 | 397 | 31.180 | 66.356 | 18.219 | 1.00 | 0.00 |
| ATOM | 1321 | CG | LYS | 2 | 397 | 32.331 | 67.372 | 18.328 | 1.00 | 0.00 |
| ATOM | 1322 | CD | LYS | 2 | 397 | 32.004 | 68.849 | 18.073 | 1.00 | 0.00 |
| ATOM | 1323 | CE | LYS | 2 | 397 | 31.159 | 69.624 | 19.086 | 1.00 | 0.00 |
| ATOM | 1324 | NZ | LYS | 2 | 397 | 30.794 | 70.914 | 18.489 | 1.00 | 0.00 |
| ATOM | 1325 | H | LYS | 2 | 397 | 32.116 | 66.523 | 15.710 | 1.00 | 0.00 |
| ATOM | 1326 | 1HZ | LYS | 2 | 397 | 30.704 | 71.662 | 19.201 | 1.00 | 0.00 |
| ATOM | 1327 | 2HZ | LYS | 2 | 397 | 31.516 | 71.194 | 17.795 | 1.00 | 0.00 |
| ATOM | 1328 | 3HZ | LYS | 2 | 397 | 29.865 | 70.849 | 18.027 | 1.00 | 0.00 |
| ATOM | 1329 | N | ASN | 2 | 398 | 29.498 | 68.230 | 15.929 | 1.00 | 0.00 |
| ATOM | 1330 | CA | ASN | 2 | 398 | 28.538 | 69.323 | 15.743 | 1.00 | 0.00 |
| ATOM | 1331 | C | ASN | 2 | 398 | 27.245 | 68.913 | 15.068 | 1.00 | 0.00 |
| ATOM | 1332 | O | ASN | 2 | 398 | 26.587 | 69.677 | 14.373 | 1.00 | 0.00 |
| ATOM | 1333 | CB | ASN | 2 | 398 | 29.153 | 70.485 | 14.962 | 1.00 | 0.00 |
| ATOM | 1334 | CG | ASN | 2 | 398 | 29.129 | 71.747 | 15.798 | 1.00 | 0.00 |
| ATOM | 1335 | OD1 | ASN | 2 | 398 | 28.125 | 72.177 | 16.357 | 1.00 | 0.00 |
| ATOM | 1336 | ND2 | ASN | 2 | 398 | 30.328 | 72.327 | 15.899 | 1.00 | 0.00 |
| ATOM | 1337 | H | ASN | 2 | 398 | 30.328 | 68.159 | 15.378 | 1.00 | 0.00 |
| ATOM | 1338 | 1HD2 | ASN | 2 | 398 | 30.447 | 73.128 | 16.481 | 1.00 | 0.00 |
| ATOM | 1339 | 2HD2 | ASN | 2 | 398 | 31.153 | 72.060 | 15.393 | 1.00 | 0.00 |
| ATOM | 1340 | N | LYS | 2 | 399 | 26.880 | 67.633 | 15.271 | 1.00 | 0.00 |
| ATOM | 1341 | CA | LYS | 2 | 399 | 25.511 | 67.187 | 15.009 | 1.00 | 0.00 |
| ATOM | 1342 | C | LYS | 2 | 399 | 24.765 | 66.868 | 16.314 | 1.00 | 0.00 |
| ATOM | 1343 | O | LYS | 2 | 399 | 23.687 | 66.280 | 16.346 | 1.00 | 0.00 |
| ATOM | 1344 | CB | LYS | 2 | 399 | 25.507 | 65.964 | 14.071 | 1.00 | 0.00 |
| ATOM | 1345 | CG | LYS | 2 | 399 | 26.746 | 65.778 | 13.173 | 1.00 | 0.00 |
| ATOM | 1346 | CD | LYS | 2 | 399 | 26.716 | 64.474 | 12.357 | 1.00 | 0.00 |
| ATOM | 1347 | CE | LYS | 2 | 399 | 28.006 | 64.151 | 11.581 | 1.00 | 0.00 |
| ATOM | 1348 | NZ | LYS | 2 | 399 | 29.028 | 63.512 | 12.413 | 1.00 | 0.00 |
| ATOM | 1349 | H | LYS | 2 | 399 | 27.521 | 67.007 | 15.710 | 1.00 | 0.00 |
| ATOM | 1350 | 1HZ | LYS | 2 | 399 | 28.967 | 63.773 | 13.417 | 1.00 | 0.00 |
| ATOM | 1351 | 2HZ | LYS | 2 | 399 | 29.021 | 62.476 | 12.283 | 1.00 | 0.00 |
| ATOM | 1352 | 3HZ | LYS | 2 | 399 | 29.939 | 63.838 | 12.060 | 1.00 | 0.00 |
| ATOM | 1353 | N | TRP | 2 | 400 | 25.438 | 67.233 | 17.425 | 1.00 | 0.00 |
| ATOM | 1354 | CA | TRP | 2 | 400 | 24.909 | 67.004 | 18.770 | 1.00 | 0.00 |
| ATOM | 1355 | C | TRP | 2 | 400 | 25.209 | 68.198 | 19.656 | 1.00 | 0.00 |
| ATOM | 1356 | O | TRP | 2 | 400 | 24.317 | 68.862 | 20.185 | 1.00 | 0.00 |
| ATOM | 1357 | CB | TRP | 2 | 400 | 25.486 | 65.728 | 19.410 | 1.00 | 0.00 |
| ATOM | 1358 | CG | TRP | 2 | 400 | 24.968 | 64.487 | 18.718 | 1.00 | 0.00 |
| ATOM | 1359 | CD1 | TRP | 2 | 400 | 23.811 | 63.760 | 19.044 | 1.00 | 0.00 |
| ATOM | 1360 | CD2 | TRP | 2 | 400 | 25.529 | 63.812 | 17.573 | 1.00 | 0.00 |
| ATOM | 1361 | NE1 | TRP | 2 | 400 | 23.627 | 62.711 | 18.194 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1362 | CE2 | TRP | 2 | 400 | 24.663 | 62.708 | 17.265 | 1.00 | 0.00 |
| ATOM | 1363 | CE3 | TRP | 2 | 400 | 26.678 | 64.047 | 16.789 | 1.00 | 0.00 |
| ATOM | 1364 | CZ2 | TRP | 2 | 400 | 24.959 | 61.873 | 16.166 | 1.00 | 0.00 |
| ATOM | 1365 | CZ3 | TRP | 2 | 400 | 26.959 | 63.200 | 15.697 | 1.00 | 0.00 |
| ATOM | 1366 | CH2 | TRP | 2 | 400 | 26.104 | 62.123 | 15.382 | 1.00 | 0.00 |
| ATOM | 1367 | H | TRP | 2 | 400 | 26.268 | 67.784 | 17.338 | 1.00 | 0.00 |
| ATOM | 1368 | HE1 | TRP | 2 | 400 | 22.898 | 62.049 | 18.223 | 1.00 | 0.00 |
| ATOM | 1369 | N | TRP | 2 | 401 | 26.522 | 68.460 | 19.766 | 1.00 | 0.00 |
| ATOM | 1370 | CA | TRP | 2 | 401 | 26.954 | 69.487 | 20.704 | 1.00 | 0.00 |
| ATOM | 1371 | C | TRP | 2 | 401 | 27.384 | 70.024 | 20.024 | 1.00 | 0.00 |
| ATOM | 1372 | O | TRP | 2 | 401 | 28.144 | 70.757 | 19.054 | 1.00 | 0.00 |
| ATOM | 1373 | CB | TRP | 2 | 401 | 28.112 | 68.970 | 21.570 | 1.00 | 0.00 |
| ATOM | 1374 | CG | TRP | 2 | 401 | 27.769 | 67.657 | 22.239 | 1.00 | 0.00 |
| ATOM | 1375 | CD1 | TRP | 2 | 401 | 26.668 | 67.394 | 23.067 | 1.00 | 0.00 |
| ATOM | 1376 | CD2 | TRP | 2 | 401 | 28.500 | 66.412 | 22.180 | 1.00 | 0.00 |
| ATOM | 1377 | NE1 | TRP | 2 | 401 | 26.673 | 66.109 | 23.508 | 1.00 | 0.00 |
| ATOM | 1378 | CE2 | TRP | 2 | 401 | 27.788 | 65.460 | 22.987 | 1.00 | 0.00 |
| ATOM | 1379 | CE3 | TRP | 2 | 401 | 29.688 | 66.026 | 21.524 | 1.00 | 0.00 |
| ATOM | 1380 | CZ2 | TRP | 2 | 401 | 28.281 | 64.145 | 23.120 | 1.00 | 0.00 |
| ATOM | 1381 | CZ3 | TRP | 2 | 401 | 30.170 | 64.707 | 21.665 | 1.00 | 0.00 |
| ATOM | 1382 | CH2 | TRP | 2 | 401 | 29.471 | 63.771 | 22.459 | 1.00 | 0.00 |
| ATOM | 1383 | H | TRP | 2 | 401 | 27.185 | 68.007 | 19.175 | 1.00 | 0.00 |
| ATOM | 1384 | HE1 | TRP | 2 | 401 | 25.987 | 65.758 | 24.126 | 1.00 | 0.00 |
| ATOM | 1385 | N | TYR | 2 | 402 | 26.915 | 71.879 | 20.627 | 1.00 | 0.00 |
| ATOM | 1386 | CA | TYR | 2 | 402 | 27.400 | 73.191 | 20.209 | 1.00 | 0.00 |
| ATOM | 1387 | C | TYR | 2 | 402 | 28.878 | 73.399 | 20.581 | 1.00 | 0.00 |
| ATOM | 1388 | O | TYR | 2 | 402 | 29.753 | 72.935 | 19.847 | 1.00 | 0.00 |
| ATOM | 1389 | CB | TYR | 2 | 402 | 26.475 | 74.310 | 20.746 | 1.00 | 0.00 |
| ATOM | 1390 | CG | TYR | 2 | 402 | 25.011 | 74.189 | 20.336 | 1.00 | 0.00 |
| ATOM | 1391 | CD1 | TYR | 2 | 402 | 24.638 | 74.314 | 18.980 | 1.00 | 0.00 |
| ATOM | 1392 | CD2 | TYR | 2 | 402 | 24.036 | 74.000 | 21.341 | 1.00 | 0.00 |
| ATOM | 1393 | CE1 | TYR | 2 | 402 | 23.272 | 74.287 | 18.632 | 1.00 | 0.00 |
| ATOM | 1394 | CE2 | TYR | 2 | 402 | 22.669 | 73.976 | 20.993 | 1.00 | 0.00 |
| ATOM | 1395 | CZ | TYR | 2 | 402 | 22.294 | 74.128 | 19.641 | 1.00 | 0.00 |
| ATOM | 1396 | OH | TYR | 2 | 402 | 20.943 | 74.106 | 19.288 | 1.00 | 0.00 |
| ATOM | 1397 | H | TYR | 2 | 402 | 26.344 | 71.829 | 21.447 | 1.00 | 0.00 |
| ATOM | 1398 | HH | TYR | 2 | 402 | 20.974 | 74.065 | 18.336 | 1.00 | 0.00 |
| ATOM | 1399 | N | ASP | 2 | 403 | 29.106 | 74.092 | 21.719 | 1.00 | 0.00 |
| ATOM | 1400 | CA | ASP | 2 | 403 | 30.498 | 74.420 | 22.060 | 1.00 | 0.00 |
| ATOM | 1401 | C | ASP | 2 | 403 | 31.161 | 73.316 | 22.869 | 1.00 | 0.00 |
| ATOM | 1402 | O | ASP | 2 | 403 | 30.495 | 72.678 | 23.690 | 1.00 | 0.00 |
| ATOM | 1403 | CB | ASP | 2 | 403 | 30.534 | 75.752 | 22.836 | 1.00 | 0.00 |
| ATOM | 1404 | CG | ASP | 2 | 403 | 31.956 | 76.263 | 23.031 | 1.00 | 0.00 |
| ATOM | 1405 | OD1 | ASP | 2 | 403 | 32.691 | 76.322 | 22.051 | 1.00 | 0.00 |
| ATOM | 1406 | OD2 | ASP | 2 | 403 | 32.331 | 76.599 | 24.154 | 1.00 | 0.00 |
| ATOM | 1407 | H | ASP | 2 | 403 | 28.387 | 74.269 | 22.386 | 1.00 | 0.00 |
| ATOM | 1408 | N | LYS | 2 | 404 | 32.469 | 73.098 | 22.639 | 1.00 | 0.00 |
| ATOM | 1409 | CA | LYS | 2 | 404 | 33.061 | 72.033 | 23.457 | 1.00 | 0.00 |
| ATOM | 1410 | C | LYS | 2 | 404 | 34.342 | 72.353 | 24.218 | 1.00 | 0.00 |
| ATOM | 1411 | O | LYS | 2 | 404 | 34.394 | 72.207 | 25.441 | 1.00 | 0.00 |
| ATOM | 1412 | CB | LYS | 2 | 404 | 33.216 | 70.687 | 22.723 | 1.00 | 0.00 |
| ATOM | 1413 | CG | LYS | 2 | 404 | 33.094 | 69.547 | 23.750 | 1.00 | 0.00 |
| ATOM | 1414 | CD | LYS | 2 | 404 | 33.852 | 68.245 | 23.463 | 1.00 | 0.00 |
| ATOM | 1415 | CE | LYS | 2 | 404 | 33.352 | 67.394 | 22.295 | 1.00 | 0.00 |
| ATOM | 1416 | NZ | LYS | 2 | 404 | 34.259 | 66.255 | 22.103 | 1.00 | 0.00 |
| ATOM | 1417 | H | LYS | 2 | 404 | 32.986 | 73.734 | 22.056 | 1.00 | 0.00 |
| ATOM | 1418 | 1HZ | LYS | 2 | 404 | 33.959 | 65.405 | 22.612 | 1.00 | 0.00 |
| ATOM | 1419 | 2HZ | LYS | 2 | 404 | 34.398 | 66.018 | 21.104 | 1.00 | 0.00 |
| ATOM | 1420 | 3HZ | LYS | 2 | 404 | 35.190 | 66.533 | 22.454 | 1.00 | 0.00 |
| ATOM | 1421 | N | GLY | 2 | 405 | 35.361 | 72.756 | 23.444 | 1.00 | 0.00 |
| ATOM | 1422 | CA | GLY | 2 | 405 | 36.660 | 73.027 | 24.065 | 1.00 | 0.00 |
| ATOM | 1423 | C | GLY | 2 | 405 | 37.572 | 71.815 | 24.165 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1424 | O | GLY | 2 | 405 | 38.013 | 71.397 | 25.240 | 1.00 | 0.00 |
| ATOM | 1425 | H | GLY | 2 | 405 | 35.233 | 72.824 | 22.455 | 1.00 | 0.00 |
| ATOM | 1426 | N | GLU | 2 | 406 | 37.858 | 71.239 | 22.988 | 1.00 | 0.00 |
| ATOM | 1427 | CA | GLU | 2 | 406 | 38.841 | 70.155 | 23.034 | 1.00 | 0.00 |
| ATOM | 1428 | C | GLU | 2 | 406 | 40.226 | 70.662 | 23.448 | 1.00 | 0.00 |
| ATOM | 1429 | O | GLU | 2 | 406 | 40.824 | 71.525 | 22.810 | 1.00 | 0.00 |
| ATOM | 1430 | CB | GLU | 2 | 406 | 38.882 | 69.401 | 21.696 | 1.00 | 0.00 |
| ATOM | 1431 | CG | GLU | 2 | 406 | 37.505 | 69.104 | 21.074 | 1.00 | 0.00 |
| ATOM | 1432 | CD | GLU | 2 | 406 | 36.885 | 67.763 | 21.460 | 1.00 | 0.00 |
| ATOM | 1433 | OE1 | GLU | 2 | 406 | 36.274 | 67.140 | 20.612 | 1.00 | 0.00 |
| ATOM | 1434 | OE2 | GLU | 2 | 406 | 36.944 | 67.309 | 22.592 | 1.00 | 0.00 |
| ATOM | 1435 | H | GLU | 2 | 406 | 37.604 | 71.743 | 22.168 | 1.00 | 0.00 |
| ATOM | 1436 | N | CYS | 2 | 407 | 40.671 | 70.094 | 24.576 | 1.00 | 0.00 |
| ATOM | 1437 | CA | CYS | 2 | 407 | 41.855 | 70.695 | 25.174 | 1.00 | 0.00 |
| ATOM | 1438 | C | CYS | 2 | 407 | 43.163 | 69.990 | 24.898 | 1.00 | 0.00 |
| ATOM | 1439 | O | CYS | 2 | 407 | 43.321 | 68.773 | 25.009 | 1.00 | 0.00 |
| ATOM | 1440 | CB | CYS | 2 | 407 | 41.654 | 70.853 | 26.678 | 1.00 | 0.00 |
| ATOM | 1441 | SG | CYS | 2 | 407 | 43.020 | 71.687 | 27.536 | 1.00 | 0.00 |
| ATOM | 1442 | H | CYS | 2 | 407 | 40.134 | 69.408 | 25.059 | 1.00 | 0.00 |
| ATOM | 1443 | N | GLY | 2 | 408 | 44.141 | 70.862 | 24.585 | 1.00 | 0.00 |
| ATOM | 1444 | CA | GLY | 2 | 408 | 45.548 | 70.490 | 24.757 | 1.00 | 0.00 |
| ATOM | 1445 | C | GLY | 2 | 408 | 45.878 | 70.421 | 26.233 | 1.00 | 0.00 |
| ATOM | 1446 | O | GLY | 2 | 408 | 46.262 | 71.391 | 26.880 | 1.00 | 0.00 |
| ATOM | 1447 | H | GLY | 2 | 408 | 43.879 | 71.819 | 24.457 | 1.00 | 0.00 |
| ATOM | 1448 | N | SER | 2 | 409 | 45.569 | 69.225 | 26.751 | 1.00 | 0.00 |
| ATOM | 1449 | CA | SER | 2 | 409 | 45.345 | 69.080 | 28.185 | 1.00 | 0.00 |
| ATOM | 1450 | C | SER | 2 | 409 | 46.609 | 68.994 | 29.024 | 1.00 | 0.00 |
| ATOM | 1451 | O | SER | 2 | 409 | 46.953 | 67.948 | 29.551 | 1.00 | 0.00 |
| ATOM | 1452 | CB | SER | 2 | 409 | 44.419 | 67.879 | 28.430 | 1.00 | 0.00 |
| ATOM | 1453 | OG | SER | 2 | 409 | 43.214 | 67.996 | 27.641 | 1.00 | 0.00 |
| ATOM | 1454 | H | SER | 2 | 409 | 45.468 | 68.466 | 26.107 | 1.00 | 0.00 |
| ATOM | 1455 | HG | SER | 2 | 409 | 43.506 | 68.029 | 26.726 | 1.00 | 0.00 |
| ATOM | 1456 | N | GLY | 2 | 410 | 47.282 | 70.150 | 29.146 | 1.00 | 0.00 |
| ATOM | 1457 | CA | GLY | 2 | 410 | 48.557 | 70.142 | 29.860 | 1.00 | 0.00 |
| ATOM | 1458 | C | GLY | 2 | 410 | 49.702 | 69.883 | 28.904 | 1.00 | 0.00 |
| ATOM | 1459 | O | GLY | 2 | 410 | 50.326 | 68.828 | 28.875 | 1.00 | 0.00 |
| ATOM | 1460 | H | GLY | 2 | 410 | 46.979 | 70.927 | 28.591 | 1.00 | 0.00 |
| ATOM | 1461 | N | GLY | 2 | 411 | 49.922 | 70.906 | 28.072 | 1.00 | 0.00 |
| ATOM | 1462 | CA | GLY | 2 | 411 | 50.778 | 70.643 | 26.922 | 1.00 | 0.00 |
| ATOM | 1463 | C | GLY | 2 | 411 | 49.984 | 69.827 | 25.928 | 1.00 | 0.00 |
| ATOM | 1464 | O | GLY | 2 | 411 | 48.825 | 70.128 | 25.666 | 1.00 | 0.00 |
| ATOM | 1465 | H | GLY | 2 | 411 | 49.363 | 71.729 | 28.131 | 1.00 | 0.00 |
| ATOM | 1466 | N | GLY | 2 | 412 | 50.636 | 68.774 | 25.425 | 1.00 | 0.00 |
| ATOM | 1467 | CA | GLY | 2 | 412 | 49.882 | 67.855 | 24.580 | 1.00 | 0.00 |
| ATOM | 1468 | C | GLY | 2 | 412 | 49.566 | 68.412 | 23.208 | 1.00 | 0.00 |
| ATOM | 1469 | O | GLY | 2 | 412 | 50.432 | 68.550 | 22.346 | 1.00 | 0.00 |
| ATOM | 1470 | H | GLY | 2 | 412 | 51.603 | 68.629 | 25.623 | 1.00 | 0.00 |
| ATOM | 1471 | N | ASP | 2 | 413 | 48.272 | 68.689 | 23.035 | 1.00 | 0.00 |
| ATOM | 1472 | CA | ASP | 2 | 413 | 47.825 | 69.187 | 21.736 | 1.00 | 0.00 |
| ATOM | 1473 | C | ASP | 2 | 413 | 48.251 | 70.636 | 21.536 | 1.00 | 0.00 |
| ATOM | 1474 | O | ASP | 2 | 413 | 48.822 | 71.269 | 22.425 | 1.00 | 0.00 |
| ATOM | 1475 | CB | ASP | 2 | 413 | 46.310 | 68.969 | 21.551 | 1.00 | 0.00 |
| ATOM | 1476 | CG | ASP | 2 | 413 | 45.970 | 67.482 | 21.524 | 1.00 | 0.00 |
| ATOM | 1477 | OD1 | ASP | 2 | 413 | 45.683 | 66.934 | 20.460 | 1.00 | 0.00 |
| ATOM | 1478 | OD2 | ASP | 2 | 413 | 46.017 | 66.816 | 22.557 | 1.00 | 0.00 |
| ATOM | 1479 | H | ASP | 2 | 413 | 47.673 | 68.730 | 23.835 | 1.00 | 0.00 |
| ATOM | 1480 | N | SER | 2 | 414 | 48.012 | 71.112 | 20.310 | 1.00 | 0.00 |
| ATOM | 1481 | CA | SER | 2 | 414 | 48.670 | 72.575 | 19.990 | 1.00 | 0.00 |
| ATOM | 1482 | C | SER | 2 | 414 | 47.878 | 73.146 | 18.965 | 1.00 | 0.00 |
| ATOM | 1483 | O | SER | 2 | 414 | 48.142 | 73.109 | 17.764 | 1.00 | 0.00 |
| ATOM | 1484 | CB | SER | 2 | 414 | 50.117 | 72.112 | 19.545 | 1.00 | 0.00 |
| ATOM | 1485 | OG | SER | 2 | 414 | 50.870 | 73.331 | 19.491 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1486 | H | SER | 2 | 414 | 47.454 | 70.606 | 19.653 | 1.00 | 0.00 |
| ATOM | 1487 | HG | SER | 2 | 414 | 50.656 | 73.720 | 18.648 | 1.00 | 0.00 |
| ATOM | 1488 | N | LYS | 2 | 415 | 46.856 | 73.813 | 19.498 | 1.00 | 0.00 |
| ATOM | 1489 | CA | LYS | 2 | 415 | 45.914 | 74.499 | 18.636 | 1.00 | 0.00 |
| ATOM | 1490 | C | LYS | 2 | 415 | 45.625 | 75.893 | 19.182 | 1.00 | 0.00 |
| ATOM | 1491 | O | LYS | 2 | 415 | 45.427 | 76.064 | 20.378 | 1.00 | 0.00 |
| ATOM | 1492 | CB | LYS | 2 | 415 | 44.647 | 73.639 | 18.527 | 1.00 | 0.00 |
| ATOM | 1493 | CG | LYS | 2 | 415 | 43.624 | 74.050 | 17.461 | 1.00 | 0.00 |
| ATOM | 1494 | CD | LYS | 2 | 415 | 42.224 | 74.241 | 18.062 | 1.00 | 0.00 |
| ATOM | 1495 | CE | LYS | 2 | 415 | 41.854 | 75.694 | 18.399 | 1.00 | 0.00 |
| ATOM | 1496 | NZ | LYS | 2 | 415 | 42.985 | 76.385 | 19.026 | 1.00 | 0.00 |
| ATOM | 1497 | OXT | LYS | 2 | 415 | 45.530 | 76.839 | 18.419 | 1.00 | 0.00 |
| ATOM | 1498 | H | LYS | 2 | 415 | 46.709 | 73.853 | 20.485 | 1.00 | 0.00 |
| ATOM | 1499 | 1HZ | LYS | 2 | 415 | 42.762 | 77.304 | 19.442 | 1.00 | 0.00 |
| ATOM | 1500 | 2HZ | LYS | 2 | 415 | 43.511 | 75.800 | 19.714 | 1.00 | 0.00 |
| ATOM | 1501 | 3HZ | LYS | 2 | 415 | 43.696 | 76.542 | 18.280 | 1.00 | 0.00 |
| ATOM | 1502 | N | SER | 1 | 1 | 47.032 | 42.057 | 10.492 | 1.00 | 0.00 |
| ATOM | 1503 | CA | SER | 1 | 1 | 47.303 | 43.393 | 11.035 | 1.00 | 0.00 |
| ATOM | 1504 | C | SER | 1 | 1 | 45.995 | 43.897 | 11.603 | 1.00 | 0.00 |
| ATOM | 1505 | O | SER | 1 | 1 | 45.273 | 43.066 | 12.151 | 1.00 | 0.00 |
| ATOM | 1506 | CB | SER | 1 | 1 | 47.891 | 44.212 | 9.881 | 1.00 | 0.00 |
| ATOM | 1507 | OG | SER | 1 | 1 | 48.673 | 43.317 | 9.061 | 1.00 | 0.00 |
| ATOM | 1508 | 1H | SER | 1 | 1 | 46.308 | 42.167 | 9.754 | 1.00 | 0.00 |
| ATOM | 1509 | 2H | SER | 1 | 1 | 47.899 | 41.688 | 10.059 | 1.00 | 0.00 |
| ATOM | 1510 | 3H | SER | 1 | 1 | 46.666 | 41.421 | 11.224 | 1.00 | 0.00 |
| ATOM | 1511 | HG | SER | 1 | 1 | 49.404 | 43.807 | 8.675 | 1.00 | 0.00 |
| ATOM | 1512 | N | SER | 1 | 2 | 45.652 | 45.188 | 11.346 | 1.00 | 0.00 |
| ATOM | 1513 | CA | SER | 1 | 2 | 44.220 | 45.473 | 11.210 | 1.00 | 0.00 |
| ATOM | 1514 | C | SER | 1 | 2 | 43.609 | 44.454 | 10.253 | 1.00 | 0.00 |
| ATOM | 1515 | O | SER | 1 | 2 | 44.146 | 44.205 | 9.173 | 1.00 | 0.00 |
| ATOM | 1516 | CB | SER | 1 | 2 | 44.005 | 46.923 | 10.745 | 1.00 | 0.00 |
| ATOM | 1517 | OG | SER | 1 | 2 | 44.631 | 47.851 | 11.662 | 1.00 | 0.00 |
| ATOM | 1518 | H | SER | 1 | 2 | 46.315 | 45.897 | 11.131 | 1.00 | 0.00 |
| ATOM | 1519 | HG | SER | 1 | 2 | 44.355 | 48.734 | 11.408 | 1.00 | 0.00 |
| ATOM | 1520 | N | GLU | 1 | 3 | 42.591 | 43.791 | 10.797 | 1.00 | 0.00 |
| ATOM | 1521 | CA | GLU | 1 | 3 | 42.407 | 42.382 | 10.459 | 1.00 | 0.00 |
| ATOM | 1522 | C | GLU | 1 | 3 | 41.603 | 42.196 | 9.171 | 1.00 | 0.00 |
| ATOM | 1523 | O | GLU | 1 | 3 | 41.620 | 43.062 | 8.294 | 1.00 | 0.00 |
| ATOM | 1524 | CB | GLU | 1 | 3 | 41.817 | 41.743 | 11.723 | 1.00 | 0.00 |
| ATOM | 1525 | CG | GLU | 1 | 3 | 42.113 | 40.280 | 12.056 | 1.00 | 0.00 |
| ATOM | 1526 | CD | GLU | 1 | 3 | 41.142 | 39.801 | 13.129 | 1.00 | 0.00 |
| ATOM | 1527 | OE1 | GLU | 1 | 3 | 40.555 | 38.740 | 12.957 | 1.00 | 0.00 |
| ATOM | 1528 | OE2 | GLU | 1 | 3 | 40.960 | 40.463 | 14.150 | 1.00 | 0.00 |
| ATOM | 1529 | H | GLU | 1 | 3 | 42.096 | 44.187 | 11.566 | 1.00 | 0.00 |
| ATOM | 1530 | N | ASN | 1 | 4 | 40.887 | 41.056 | 9.065 | 1.00 | 0.00 |
| ATOM | 1531 | CA | ASN | 1 | 4 | 39.950 | 41.050 | 7.941 | 1.00 | 0.00 |
| ATOM | 1532 | C | ASN | 1 | 4 | 38.711 | 41.864 | 8.303 | 1.00 | 0.00 |
| ATOM | 1533 | O | ASN | 1 | 4 | 38.269 | 42.742 | 7.566 | 1.00 | 0.00 |
| ATOM | 1534 | CB | ASN | 1 | 4 | 39.643 | 39.620 | 7.453 | 1.00 | 0.00 |
| ATOM | 1535 | CG | ASN | 1 | 4 | 39.405 | 39.557 | 5.939 | 1.00 | 0.00 |
| ATOM | 1536 | OD1 | ASN | 1 | 4 | 39.976 | 38.757 | 5.203 | 1.00 | 0.00 |
| ATOM | 1537 | ND2 | ASN | 1 | 4 | 38.475 | 40.408 | 5.484 | 1.00 | 0.00 |
| ATOM | 1538 | H | ASN | 1 | 4 | 40.809 | 40.427 | 9.834 | 1.00 | 0.00 |
| ATOM | 1539 | 1HD2 | ASN | 1 | 4 | 38.246 | 40.274 | 4.521 | 1.00 | 0.00 |
| ATOM | 1540 | 2HD2 | ASN | 1 | 4 | 38.028 | 41.112 | 6.038 | 1.00 | 0.00 |
| ATOM | 1541 | N | ARG | 1 | 5 | 38.209 | 41.597 | 9.521 | 1.00 | 0.00 |
| ATOM | 1542 | CA | ARG | 1 | 5 | 37.366 | 42.620 | 10.140 | 1.00 | 0.00 |
| ATOM | 1543 | C | ARG | 1 | 5 | 38.061 | 43.092 | 11.403 | 1.00 | 0.00 |
| ATOM | 1544 | O | ARG | 1 | 5 | 38.982 | 42.450 | 11.979 | 1.00 | 0.00 |
| ATOM | 1545 | CB | ARG | 1 | 5 | 35.963 | 42.101 | 10.485 | 1.00 | 0.00 |
| ATOM | 1546 | CG | ARG | 1 | 5 | 35.150 | 41.522 | 9.320 | 1.00 | 0.00 |
| ATOM | 1547 | CD | ARG | 1 | 5 | 34.826 | 42.488 | 8.168 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1548 | NE | ARG | 1 | 5 | 33.966 | 43.612 | 8.557 | 1.00 | 0.00 |
| ATOM | 1549 | CZ | ARG | 1 | 5 | 32.613 | 43.507 | 8.590 | 1.00 | 0.00 |
| ATOM | 1550 | NH1 | ARG | 1 | 5 | 31.306 | 44.603 | 8.845 | 1.00 | 0.00 |
| ATOM | 1551 | NH2 | ARG | 1 | 5 | 31.978 | 42.355 | 8.395 | 1.00 | 0.00 |
| ATOM | 1552 | H | ARG | 1 | 5 | 38.562 | 40.873 | 10.117 | 1.00 | 0.00 |
| ATOM | 1553 | HE | ARG | 1 | 5 | 34.360 | 44.527 | 8.685 | 1.00 | 0.00 |
| ATOM | 1554 | 1HH1 | ARG | 1 | 5 | 30.903 | 44.563 | 8.878 | 1.00 | 0.00 |
| ATOM | 1555 | 2HH1 | ARG | 1 | 5 | 32.339 | 45.497 | 9.006 | 1.00 | 0.00 |
| ATOM | 1556 | 1HH2 | ARG | 1 | 5 | 30.975 | 42.325 | 8.443 | 1.00 | 0.00 |
| ATOM | 1557 | 2HH2 | ARG | 1 | 5 | 32.464 | 41.509 | 8.198 | 1.00 | 0.00 |
| ATOM | 1558 | N | THR | 1 | 6 | 37.630 | 44.240 | 11.923 | 1.00 | 0.00 |
| ATOM | 1559 | CA | THR | 1 | 6 | 38.078 | 44.601 | 13.272 | 1.00 | 0.00 |
| ATOM | 1560 | C | THR | 1 | 6 | 36.953 | 45.404 | 13.890 | 1.00 | 0.00 |
| ATOM | 1561 | O | THR | 1 | 6 | 36.277 | 46.127 | 13.150 | 1.00 | 0.00 |
| ATOM | 1562 | CB | THR | 1 | 6 | 39.404 | 45.370 | 13.322 | 1.00 | 0.00 |
| ATOM | 1563 | OG1 | THR | 1 | 6 | 40.179 | 44.957 | 12.078 | 1.00 | 0.00 |
| ATOM | 1564 | CG2 | THR | 1 | 6 | 40.215 | 45.127 | 14.494 | 1.00 | 0.00 |
| ATOM | 1565 | H | THR | 1 | 6 | 36.926 | 44.787 | 11.480 | 1.00 | 0.00 |
| ATOM | 1566 | HG1 | THR | 1 | 6 | 40.113 | 43.999 | 12.080 | 1.00 | 0.00 |
| ATOM | 1567 | N | ILE | 1 | 7 | 36.664 | 45.177 | 15.173 | 1.00 | 0.00 |
| ATOM | 1568 | CA | ILE | 1 | 7 | 35.285 | 45.481 | 15.574 | 1.00 | 0.00 |
| ATOM | 1569 | C | ILE | 1 | 7 | 35.103 | 46.750 | 16.418 | 1.00 | 0.00 |
| ATOM | 1570 | O | ILE | 1 | 7 | 35.844 | 47.042 | 17.360 | 1.00 | 0.00 |
| ATOM | 1571 | CB | ILE | 1 | 7 | 34.716 | 44.203 | 16.225 | 1.00 | 0.00 |
| ATOM | 1572 | CG1 | ILE | 1 | 7 | 34.863 | 42.999 | 15.286 | 1.00 | 0.00 |
| ATOM | 1573 | CG2 | ILE | 1 | 7 | 33.258 | 44.332 | 16.677 | 1.00 | 0.00 |
| ATOM | 1574 | CD1 | ILE | 1 | 7 | 34.493 | 41.659 | 15.928 | 1.00 | 0.00 |
| ATOM | 1575 | H | ILE | 1 | 7 | 37.296 | 44.708 | 15.797 | 1.00 | 0.00 |
| ATOM | 1576 | N | VAL | 1 | 8 | 34.076 | 47.518 | 16.032 | 1.00 | 0.00 |
| ATOM | 1577 | CA | VAL | 1 | 8 | 33.654 | 48.559 | 16.961 | 1.00 | 0.00 |
| ATOM | 1578 | C | VAL | 1 | 8 | 32.665 | 47.952 | 17.917 | 1.00 | 0.00 |
| ATOM | 1579 | O | VAL | 1 | 8 | 31.543 | 47.672 | 17.520 | 1.00 | 0.00 |
| ATOM | 1580 | CB | VAL | 1 | 8 | 33.015 | 49.706 | 16.170 | 1.00 | 0.00 |
| ATOM | 1581 | CG1 | VAL | 1 | 8 | 32.197 | 50.704 | 16.994 | 1.00 | 0.00 |
| ATOM | 1582 | CG2 | VAL | 1 | 8 | 34.117 | 50.416 | 15.411 | 1.00 | 0.00 |
| ATOM | 1583 | H | VAL | 1 | 8 | 33.477 | 47.180 | 15.313 | 1.00 | 0.00 |
| ATOM | 1584 | N | VAL | 1 | 9 | 33.095 | 47.729 | 19.159 | 1.00 | 0.00 |
| ATOM | 1585 | CA | VAL | 1 | 9 | 31.987 | 47.430 | 20.053 | 1.00 | 0.00 |
| ATOM | 1586 | C | VAL | 1 | 9 | 31.515 | 48.668 | 20.762 | 1.00 | 0.00 |
| ATOM | 1587 | O | VAL | 1 | 9 | 32.161 | 49.710 | 20.749 | 1.00 | 0.00 |
| ATOM | 1588 | CB | VAL | 1 | 9 | 32.249 | 46.273 | 21.025 | 1.00 | 0.00 |
| ATOM | 1589 | CG1 | VAL | 1 | 9 | 32.126 | 44.957 | 20.264 | 1.00 | 0.00 |
| ATOM | 1590 | CG2 | VAL | 1 | 9 | 33.547 | 46.405 | 21.823 | 1.00 | 0.00 |
| ATOM | 1591 | H | VAL | 1 | 9 | 34.023 | 47.889 | 19.488 | 1.00 | 0.00 |
| ATOM | 1592 | N | THR | 1 | 10 | 30.351 | 48.510 | 21.380 | 1.00 | 0.00 |
| ATOM | 1593 | CA | THR | 1 | 10 | 29.656 | 49.641 | 21.970 | 1.00 | 0.00 |
| ATOM | 1594 | C | THR | 1 | 10 | 28.529 | 49.125 | 22.832 | 1.00 | 0.00 |
| ATOM | 1595 | O | THR | 1 | 10 | 28.137 | 47.956 | 22.782 | 1.00 | 0.00 |
| ATOM | 1596 | CB | THR | 1 | 10 | 29.133 | 50.582 | 20.864 | 1.00 | 0.00 |
| ATOM | 1597 | OG1 | THR | 1 | 10 | 28.571 | 51.785 | 21.420 | 1.00 | 0.00 |
| ATOM | 1598 | CG2 | THR | 1 | 10 | 28.131 | 49.918 | 19.912 | 1.00 | 0.00 |
| ATOM | 1599 | H | THR | 1 | 10 | 29.880 | 47.636 | 21.310 | 1.00 | 0.00 |
| ATOM | 1600 | HG1 | THR | 1 | 10 | 28.750 | 52.452 | 20.747 | 1.00 | 0.00 |
| ATOM | 1601 | N | THR | 1 | 11 | 27.992 | 50.044 | 23.634 | 1.00 | 0.00 |
| ATOM | 1602 | CA | THR | 1 | 11 | 26.693 | 49.704 | 24.190 | 1.00 | 0.00 |
| ATOM | 1603 | C | THR | 1 | 11 | 25.599 | 50.734 | 23.937 | 1.00 | 0.00 |
| ATOM | 1604 | O | THR | 1 | 11 | 25.038 | 51.364 | 24.829 | 1.00 | 0.00 |
| ATOM | 1605 | CB | THR | 1 | 11 | 26.793 | 49.340 | 25.665 | 1.00 | 0.00 |
| ATOM | 1606 | OG1 | THR | 1 | 11 | 28.031 | 48.651 | 25.977 | 1.00 | 0.00 |
| ATOM | 1607 | CG2 | THR | 1 | 11 | 25.566 | 48.494 | 26.025 | 1.00 | 0.00 |
| ATOM | 1608 | H | THR | 1 | 11 | 28.360 | 50.968 | 23.714 | 1.00 | 0.00 |
| ATOM | 1609 | HG1 | THR | 1 | 11 | 28.083 | 47.958 | 25.314 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1610 | N | ILE | 1 | 12 | 25.241 | 50.640 | 22.645 | 1.00 | 0.00 |
| ATOM | 1611 | CA | ILE | 1 | 12 | 34.187 | 51.750 | 11.164 | 1.00 | 0.00 |
| ATOM | 1612 | C | ILE | 1 | 12 | 22.235 | 51.998 | 23.044 | 1.00 | 0.00 |
| ATOM | 1613 | O | ILE | 1 | 12 | 22.279 | 53.039 | 23.011 | 1.00 | 0.00 |
| ATOM | 1614 | CB | ILE | 1 | 12 | 23.924 | 51.283 | 20.748 | 1.00 | 0.00 |
| ATOM | 1615 | CG1 | ILE | 1 | 12 | 22.875 | 52.249 | 20.042 | 1.00 | 0.00 |
| ATOM | 1616 | CG2 | ILE | 1 | 12 | 23.270 | 49.851 | 20.802 | 1.00 | 0.00 |
| ATOM | 1617 | CD1 | ILE | 1 | 12 | 22.271 | 51.637 | 18.787 | 1.00 | 0.00 |
| ATOM | 1618 | H | ILE | 1 | 12 | 25.862 | 50.401 | 22.001 | 1.00 | 0.00 |
| ATOM | 1619 | N | LEU | 1 | 13 | 22.644 | 50.991 | 23.889 | 1.00 | 0.00 |
| ATOM | 1620 | CA | LEU | 1 | 13 | 21.737 | 51.155 | 25.035 | 1.00 | 0.00 |
| ATOM | 1621 | C | LEU | 1 | 13 | 21.885 | 52.423 | 25.898 | 1.00 | 0.00 |
| ATOM | 1622 | O | LEU | 1 | 13 | 20.979 | 52.830 | 26.631 | 1.00 | 0.00 |
| ATOM | 1623 | CB | LEU | 1 | 13 | 21.860 | 49.895 | 25.900 | 1.00 | 0.00 |
| ATOM | 1624 | CG | LEU | 1 | 13 | 20.779 | 49.677 | 26.963 | 1.00 | 0.00 |
| ATOM | 1625 | CD1 | LEU | 1 | 13 | 19.418 | 49.351 | 26.347 | 1.00 | 0.00 |
| ATOM | 1626 | CD2 | LEU | 1 | 13 | 21.205 | 48/620 | 27.982 | 1.00 | 0.00 |
| ATOM | 1627 | H | LEU | 1 | 13 | 23.163 | 50.143 | 23.796 | 1.00 | 0.00 |
| ATOM | 1628 | N | GLU | 1 | 14 | 23.071 | 53.038 | 25.818 | 1.00 | 0.00 |
| ATOM | 1629 | CA | GLU | 1 | 14 | 23.379 | 54.247 | 26.581 | 1.00 | 0.00 |
| ATOM | 1630 | C | GLU | 1 | 14 | 22.920 | 55.529 | 25.891 | 1.00 | 0.00 |
| ATOM | 1631 | O | GLU | 1 | 14 | 22.182 | 55.537 | 24.907 | 1.00 | 0.00 |
| ATOM | 1632 | CB | GLU | 1 | 14 | 24.893 | 54.295 | 26.818 | 1.00 | 0.00 |
| ATOM | 1633 | CG | GLU | 1 | 14 | 25.478 | 53.048 | 27.490 | 1.00 | 0.00 |
| ATOM | 1634 | CD | GLU | 1 | 14 | 26.826 | 52.694 | 26.873 | 1.00 | 0.00 |
| ATOM | 1635 | OE1 | GLU | 1 | 14 | 27.621 | 52.029 | 27.532 | 1.00 | 0.00 |
| ATOM | 1636 | OE2 | GLU | 1 | 14 | 27.084 | 53.050 | 25.723 | 1.00 | 0.00 |
| ATOM | 1637 | H | GLU | 1 | 14 | 23.745 | 52.673 | 25.183 | 1.00 | 0.00 |
| ATOM | 1638 | N | SER | 1 | 15 | 23.429 | 56/635 | 26.429 | 1.00 | 0.00 |
| ATOM | 1639 | CA | SER | 1 | 15 | 23.322 | 57.982 | 25.688 | 1.00 | 0.00 |
| ATOM | 1640 | C | SER | 1 | 15 | 24.619 | 58.623 | 25.922 | 1.00 | 0.00 |
| ATOM | 1641 | O | SER | 1 | 15 | 25.236 | 58.447 | 26.974 | 1.00 | 0.00 |
| ATOM | 1642 | CB | SER | 1 | 15 | 23.106 | 58.664 | 26.175 | 1.00 | 0.00 |
| ATOM | 1643 | OG | SER | 1 | 15 | 20.982 | 57.777 | 26.322 | 1.00 | 0.00 |
| ATOM | 1644 | H | SER | 1 | 15 | 24.032 | 56.624 | 27.230 | 1.00 | 0.00 |
| ATOM | 1645 | HG | SER | 1 | 15 | 21.014 | 57.190 | 25.566 | 1.00 | 0.00 |
| ATOM | 1646 | N | PRO | 1 | 16 | 25.077 | 59.453 | 24.950 | 1.00 | 0.00 |
| ATOM | 1647 | CA | PRO | 1 | 16 | 24.267 | 59.970 | 23.837 | 1.00 | 0.00 |
| ATOM | 1648 | C | PRO | 1 | 16 | 24.185 | 59.219 | 22.518 | 1.00 | 0.00 |
| ATOM | 1649 | O | PRO | 1 | 16 | 23.929 | 59.885 | 21.515 | 1.00 | 0.00 |
| ATOM | 1650 | CB | PRO | 1 | 16 | 24.904 | 61.344 | 23.610 | 1.00 | 0.00 |
| ATOM | 1651 | CG | PRO | 1 | 16 | 26.383 | 61.125 | 23.849 | 1.00 | 0.00 |
| ATOM | 1652 | CD | PRO | 1 | 16 | 26.365 | 60.134 | 25.051 | 1.00 | 0.00 |
| ATOM | 1653 | N | TYR | 1 | 17 | 24.397 | 57.898 | 22.466 | 1.00 | 0.00 |
| ATOM | 1654 | CA | TYR | 1 | 17 | 24.621 | 57.373 | 21.108 | 1.00 | 0.00 |
| ATOM | 1655 | C | TYR | 1 | 17 | 23.441 | 56.977 | 20.212 | 1.00 | 0.00 |
| ATOM | 1656 | O | TYR | 1 | 17 | 23.176 | 55.836 | 19.816 | 1.00 | 0.00 |
| ATOM | 1657 | CB | TYR | 1 | 17 | 25.821 | 56.419 | 21.125 | 1.00 | 0.00 |
| ATOM | 1658 | CG | TYR | 1 | 17 | 27.001 | 57.257 | 21.573 | 1.00 | 0.00 |
| ATOM | 1659 | CD1 | TYR | 1 | 17 | 27.470 | 58.286 | 20.727 | 1.00 | 0.00 |
| ATOM | 1660 | CD2 | TYR | 1 | 17 | 27.557 | 57.041 | 22.850 | 1.00 | 0.00 |
| ATOM | 1661 | CE1 | TYR | 1 | 17 | 28.413 | 59.203 | 21.216 | 1.00 | 0.00 |
| ATOM | 1662 | CE2 | TYR | 1 | 17 | 28.494 | 57.964 | 23.343 | 1.00 | 0.00 |
| ATOM | 1663 | CZ | TYR | 1 | 17 | 28.859 | 59.070 | 22.545 | 1.00 | 0.00 |
| ATOM | 1664 | OH | TYR | 1 | 17 | 29.631 | 60.075 | 23.106 | 1.00 | 0.00 |
| ATOM | 1665 | H | TYR | 1 | 17 | 24.543 | 57.337 | 23.280 | 1.00 | 0.00 |
| ATOM | 1666 | HH | TYR | 1 | 17 | 30.011 | 60.589 | 22.388 | 1.00 | 0.00 |
| ATOM | 1667 | N | VAL | 1 | 18 | 22.736 | 58.066 | 19.862 | 1.00 | 0.00 |
| ATOM | 1668 | CA | VAL | 1 | 18 | 21.481 | 58.122 | 19.118 | 1.00 | 0.00 |
| ATOM | 1669 | C | VAL | 1 | 18 | 20.510 | 56.982 | 19.373 | 1.00 | 0.00 |
| ATOM | 1670 | O | VAL | 1 | 18 | 19.870 | 56.455 | 18.466 | 1.00 | 0.00 |
| ATOM | 1671 | CB | VAL | 1 | 18 | 21.722 | 58.395 | 17.618 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1672 | CG1 | VAL | 1 | 18 | 20.470 | 58.900 | 16.886 | 1.00 | 0.00 |
| ATOM | 1673 | CG2 | VAL | 1 | 18 | 22.818 | 59.442 | 17.448 | 1.00 | 0.00 |
| ATOM | 1674 | H | VAL | 1 | 18 | 23.172 | 58.919 | 20.124 | 1.00 | 0.00 |
| ATOM | 1675 | N | MET | 1 | 19 | 20.416 | 56.646 | 20.672 | 1.00 | 0.00 |
| ATOM | 1676 | CA | MET | 1 | 19 | 19.411 | 55.729 | 21.218 | 1.00 | 0.00 |
| ATOM | 1677 | C | MET | 1 | 19 | 19.359 | 54.357 | 20.571 | 1.00 | 0.00 |
| ATOM | 1678 | O | MET | 1 | 19 | 19.385 | 54.196 | 19.355 | 1.00 | 0.00 |
| ATOM | 1679 | CB | MET | 1 | 19 | 18.003 | 56.342 | 21.267 | 1.00 | 0.00 |
| ATOM | 1680 | CG | MET | 1 | 19 | 19.919 | 57.710 | 21.953 | 1.00 | 0.00 |
| ATOM | 1681 | SD | MET | 1 | 19 | 18.451 | 59.057 | 20.883 | 1.00 | 0.00 |
| ATOM | 1682 | CE | MET | 1 | 19 | 18.605 | 60.345 | 22.130 | 1.00 | 0.00 |
| ATOM | 1683 | H | MET | 1 | 19 | 21.226 | 56.864 | 21.212 | 1.00 | 0.00 |
| ATOM | 1684 | N | TYR | 1 | 20 | 19.296 | 53.346 | 21.445 | 1.00 | 0.00 |
| ATOM | 1685 | CA | TYR | 1 | 20 | 19.315 | 51.963 | 20.950 | 1.00 | 0.00 |
| ATOM | 1686 | C | TYR | 1 | 20 | 18.288 | 51.589 | 19.886 | 1.00 | 0.00 |
| ATOM | 1687 | O | TYR | 1 | 20 | 17.138 | 51.230 | 20.150 | 1.00 | 0.00 |
| ATOM | 1688 | CB | TYR | 1 | 20 | 19.332 | 50.953 | 22.115 | 1.00 | 0.00 |
| ATOM | 1689 | CG | TYR | 1 | 20 | 18.214 | 51.159 | 23.121 | 1.00 | 0.00 |
| ATOM | 1690 | CD1 | TYR | 1 | 20 | 18.376 | 52.114 | 24.147 | 1.00 | 0.00 |
| ATOM | 1691 | CD2 | TYR | 1 | 20 | 17.046 | 50.374 | 23.021 | 1.00 | 0.00 |
| ATOM | 1692 | CE1 | TYR | 1 | 20 | 17.354 | 52.284 | 25.094 | 1.00 | 0.00 |
| ATOM | 1693 | CE2 | TYR | 1 | 20 | 16.021 | 50.546 | 23.966 | 1.00 | 0.00 |
| ATOM | 1694 | CZ | TYR | 1 | 20 | 16.191 | 51.495 | 24.993 | 1.00 | 0.00 |
| ATOM | 1695 | OH | TYR | 1 | 20 | 15.188 | 51.659 | 25.933 | 1.00 | 0.00 |
| ATOM | 1696 | H | TYR | 1 | 20 | 19.220 | 53.552 | 22.422 | 1.00 | 0.00 |
| ATOM | 1697 | HH | TYR | 1 | 20 | 15.558 | 52.069 | 26.713 | 1.00 | 0.00 |
| ATOM | 1698 | N | LYS | 1 | 21 | 18.727 | 51.670 | 18.624 | 1.00 | 0.00 |
| ATOM | 1699 | CA | LYS | 1 | 21 | 17.745 | 51.259 | 17.625 | 1.00 | 0.00 |
| ATOM | 1700 | C | LYS | 1 | 21 | 17.992 | 49.942 | 16.934 | 1.00 | 0.00 |
| ATOM | 1701 | O | LYS | 1 | 21 | 18.054 | 49.887 | 15.704 | 1.00 | 0.00 |
| ATOM | 1702 | CB | LYS | 1 | 21 | 17.437 | 52.349 | 16.592 | 1.00 | 0.00 |
| ATOM | 1703 | CG | LYS | 1 | 21 | 15.937 | 52.679 | 16.506 | 1.00 | 0.00 |
| ATOM | 1704 | CD | LYS | 1 | 21 | 14.952 | 51.545 | 16.153 | 1.00 | 0.00 |
| ATOM | 1705 | CE | LYS | 1 | 21 | 14.897 | 51.094 | 14.683 | 1.00 | 0.00 |
| ATOM | 1706 | NZ | LYS | 1 | 21 | 15.716 | 49.900 | 14.443 | 1.00 | 0.00 |
| ATOM | 1707 | H | LYS | 1 | 21 | 19.656 | 52.013 | 18.458 | 1.00 | 0.00 |
| ATOM | 1708 | 1HZ | LYS | 1 | 21 | 15.348 | 49.074 | 14.964 | 1.00 | 0.00 |
| ATOM | 1709 | 2HZ | LYS | 1 | 21 | 15.676 | 49.651 | 13.434 | 1.00 | 0.00 |
| ATOM | 1710 | 3HZ | LYS | 1 | 21 | 16.712 | 50.016 | 14.713 | 1.00 | 0.00 |
| ATOM | 1711 | N | LYS | 1 | 22 | 18.041 | 48.882 | 17.756 | 1.00 | 0.00 |
| ATOM | 1712 | CA | LYS | 1 | 22 | 18.132 | 47.532 | 17.195 | 1.00 | 0.00 |
| ATOM | 1713 | C | LYS | 1 | 22 | 17.219 | 47.259 | 16.006 | 1.00 | 0.00 |
| ATOM | 1714 | O | LYS | 1 | 22 | 16.132 | 47.823 | 15.857 | 1.00 | 0.00 |
| ATOM | 1715 | CB | LYS | 1 | 22 | 17.979 | 46.475 | 18.295 | 1.00 | 0.00 |
| ATOM | 1716 | CG | LYS | 1 | 22 | 19.071 | 46.479 | 19.381 | 1.00 | 0.00 |
| ATOM | 1717 | CD | LYS | 1 | 22 | 20.492 | 46.228 | 18.857 | 1.00 | 0.00 |
| ATOM | 1718 | CE | LYS | 1 | 22 | 21.309 | 47.508 | 18.649 | 1.00 | 0.00 |
| ATOM | 1719 | NZ | LYS | 1 | 22 | 22.256 | 47.317 | 17.552 | 1.00 | 0.00 |
| ATOM | 1720 | H | LYS | 1 | 22 | 18.006 | 49.036 | 18.743 | 1.00 | 0.00 |
| ATOM | 1721 | 1HZ | LYS | 1 | 22 | 21.759 | 46.903 | 16.740 | 1.00 | 0.00 |
| ATOM | 1722 | 2HZ | LYS | 1 | 22 | 22.627 | 48.226 | 17.222 | 1.00 | 0.00 |
| ATOM | 1723 | 3HZ | LYS | 1 | 22 | 23.007 | 46.635 | 17.766 | 1.00 | 0.00 |
| ATOM | 1724 | N | ASN | 1 | 23 | 17.786 | 46.448 | 15.112 | 1.00 | 0.00 |
| ATOM | 1725 | CA | ASN | 1 | 23 | 17.265 | 46.271 | 13.758 | 1.00 | 0.00 |
| ATOM | 1726 | C | ASN | 1 | 23 | 17.549 | 44.849 | 13.326 | 1.00 | 0.00 |
| ATOM | 1727 | O | ASN | 1 | 23 | 18.050 | 44.078 | 14.139 | 1.00 | 0.00 |
| ATOM | 1728 | CB | ASN | 1 | 23 | 17.952 | 47.248 | 12.807 | 1.00 | 0.00 |
| ATOM | 1729 | CG | ASN | 1 | 23 | 16.941 | 47.818 | 11.851 | 1.00 | 0.00 |
| ATOM | 1730 | OD1 | ASN | 1 | 23 | 16.014 | 48.506 | 12.281 | 1.00 | 0.00 |
| ATOM | 1731 | ND2 | ASN | 1 | 23 | 17.150 | 47.542 | 10.563 | 1.00 | 0.00 |
| ATOM | 1732 | H | ASN | 1 | 23 | 18.639 | 46.946 | 15.301 | 1.00 | 0.00 |
| ATOM | 1733 | 1HD2 | ASN | 1 | 23 | 16.536 | 47.864 | 9.846 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1734 | 2HD2 | ASN | 1 | 23 | 17.943 | 47.012 | 10.235 | 1.00 | 0.00 |
| ATOM | 1735 | N | ASN | 1 | 24 | 17.235 | 44.535 | 12.058 | 1.00 | 0.00 |
| ATOM | 1736 | CA | ASN | 1 | 24 | 17.395 | 43.143 | 11.634 | 1.00 | 0.00 |
| ATOM | 1737 | C | ASN | 1 | 24 | 17.212 | 42.912 | 10.147 | 1.00 | 0.00 |
| ATOM | 1738 | O | ASN | 1 | 24 | 16.276 | 42.251 | 9.709 | 1.00 | 0.00 |
| ATOM | 1739 | CB | ASN | 1 | 24 | 16.454 | 42.213 | 12.405 | 1.00 | 0.00 |
| ATOM | 1740 | CG | ASN | 1 | 24 | 17.134 | 40.878 | 12.591 | 1.00 | 0.00 |
| ATOM | 1741 | OD1 | ASN | 1 | 24 | 16.721 | 39.864 | 12.041 | 1.00 | 0.00 |
| ATOM | 1742 | ND2 | ASN | 1 | 24 | 18.176 | 40.914 | 13.430 | 1.00 | 0.00 |
| ATOM | 1743 | H | ASN | 1 | 24 | 16.913 | 45.204 | 11.392 | 1.00 | 0.00 |
| ATOM | 1744 | 1HD2 | ASN | 1 | 24 | 18.661 | 40.058 | 13.588 | 1.00 | 0.00 |
| ATOM | 1745 | 2HD2 | ASN | 1 | 24 | 18.410 | 41.784 | 13.866 | 1.00 | 0.00 |
| ATOM | 1746 | N | GLU | 1 | 25 | 18.139 | 43.499 | 9.374 | 1.00 | 0.00 |
| ATOM | 1747 | CA | GLU | 1 | 25 | 18.167 | 43.086 | 7.976 | 1.00 | 0.00 |
| ATOM | 1748 | C | GLU | 1 | 25 | 19.137 | 41.926 | 7.840 | 1.00 | 0.00 |
| ATOM | 1749 | O | GLU | 1 | 25 | 20.062 | 41.814 | 8.643 | 1.00 | 0.00 |
| ATOM | 1750 | CB | GLU | 1 | 25 | 18.498 | 44.286 | 7.071 | 1.00 | 0.00 |
| ATOM | 1751 | CG | GLU | 1 | 25 | 19.914 | 44.890 | 7.119 | 1.00 | 0.00 |
| ATOM | 1752 | CD | GLU | 1 | 25 | 20.307 | 45.419 | 8.491 | 1.00 | 0.00 |
| ATOM | 1753 | OE1 | GLU | 1 | 25 | 19.564 | 46.177 | 9.109 | 1.00 | 0.00 |
| ATOM | 1754 | OE2 | GLU | 1 | 25 | 21.384 | 45.076 | 8.951 | 1.00 | 0.00 |
| ATOM | 1755 | H | GLU | 1 | 25 | 18.875 | 44.054 | 9.732 | 1.00 | 0.00 |
| ATOM | 1756 | N | GLN | 1 | 26 | 18.889 | 41.056 | 6.847 | 1.00 | 0.00 |
| ATOM | 1757 | CA | GLN | 1 | 26 | 19.531 | 39.732 | 6.876 | 1.00 | 0.00 |
| ATOM | 1758 | C | GLN | 1 | 26 | 20.990 | 39.626 | 6.429 | 1.00 | 0.00 |
| ATOM | 1759 | O | GLN | 1 | 26 | 21.390 | 36.658 | 5.778 | 1.00 | 0.00 |
| ATOM | 1760 | CB | GLN | 1 | 26 | 18.678 | 38.708 | 6.110 | 1.00 | 0.00 |
| ATOM | 1761 | CG | GLN | 1 | 26 | 17.339 | 38.316 | 6.753 | 1.00 | 0.00 |
| ATOM | 1762 | CD | GLN | 1 | 26 | 16.354 | 39.469 | 6.735 | 1.00 | 0.00 |
| ATOM | 1763 | OE1 | GLN | 1 | 26 | 15.833 | 39.880 | 5.703 | 1.00 | 0.00 |
| ATOM | 1764 | NE2 | GLN | 1 | 26 | 16.130 | 39.992 | 7.938 | 1.00 | 0.00 |
| ATOM | 1765 | H | GLN | 1 | 26 | 18.174 | 41.239 | 6.166 | 1.00 | 0.00 |
| ATOM | 1766 | 1HE2 | GLN | 1 | 26 | 15.545 | 40.858 | 8.058 | 1.00 | 0.00 |
| ATOM | 1767 | 2HE2 | GLN | 1 | 26 | 16.516 | 39.503 | 8.773 | 1.00 | 0.00 |
| ATOM | 1768 | N | LEU | 1 | 27 | 21.758 | 40.668 | 6.807 | 1.00 | 0.00 |
| ATOM | 1769 | CA | LEU | 1 | 27 | 23.168 | 40.720 | 6.433 | 1.00 | 0.00 |
| ATOM | 1770 | C | LEU | 1 | 27 | 23.968 | 41.690 | 7.297 | 1.00 | 0.00 |
| ATOM | 1771 | O | LEU | 1 | 27 | 24.972 | 42.250 | 6.873 | 1.00 | 0.00 |
| ATOM | 1772 | CB | LEU | 1 | 27 | 23.305 | 41.074 | 4.943 | 1.00 | 0.00 |
| ATOM | 1773 | CG | LEU | 1 | 27 | 24.609 | 40.598 | 4.290 | 1.00 | 0.00 |
| ATOM | 1774 | CD1 | LEU | 1 | 27 | 24.776 | 39.079 | 4.375 | 1.00 | 0.00 |
| ATOM | 1775 | CD2 | LEU | 1 | 27 | 24.736 | 41.109 | 2.854 | 1.00 | 0.00 |
| ATOM | 1776 | H | LEU | 1 | 27 | 21.320 | 41.404 | 7.315 | 1.00 | 0.00 |
| ATOM | 1777 | N | GLU | 1 | 28 | 23.459 | 41.914 | 8.527 | 1.00 | 0.00 |
| ATOM | 1778 | CA | GLU | 1 | 28 | 24.060 | 42.782 | 9.563 | 1.00 | 0.00 |
| ATOM | 1779 | C | GLU | 1 | 28 | 24.309 | 44.273 | 9.326 | 1.00 | 0.00 |
| ATOM | 1780 | O | GLU | 1 | 28 | 24.505 | 45.044 | 10.264 | 1.00 | 0.00 |
| ATOM | 1781 | CB | GLU | 1 | 28 | 25.308 | 42.151 | 10.214 | 1.00 | 0.00 |
| ATOM | 1782 | CG | GLU | 1 | 28 | 26.698 | 42.480 | 9.617 | 1.00 | 0.00 |
| ATOM | 1783 | CD | GLU | 1 | 28 | 27.790 | 41.758 | 10.395 | 1.00 | 0.00 |
| ATOM | 1784 | OE1 | GLU | 1 | 28 | 27.508 | 40.723 | 10.973 | 1.00 | 0.00 |
| ATOM | 1785 | OE2 | GLU | 1 | 28 | 28.935 | 42.207 | 10.450 | 1.00 | 0.00 |
| ATOM | 1786 | H | GLU | 1 | 28 | 22.645 | 41.390 | 8.783 | 1.00 | 0.00 |
| ATOM | 1787 | N | GLY | 1 | 29 | 24.348 | 44.650 | 8.038 | 1.00 | 0.00 |
| ATOM | 1788 | CA | GLY | 1 | 29 | 24.998 | 45.904 | 7.666 | 1.00 | 0.00 |
| ATOM | 1789 | C | GLY | 1 | 29 | 24.547 | 47.150 | 8.405 | 1.00 | 0.00 |
| ATOM | 1790 | O | GLY | 1 | 29 | 25.358 | 47.972 | 8.842 | 1.00 | 0.00 |
| ATOM | 1791 | H | GLY | 1 | 29 | 24.153 | 43.954 | 7.355 | 1.00 | 0.00 |
| ATOM | 1792 | N | ASN | 1 | 30 | 23.212 | 47.263 | 8.472 | 1.00 | 0.00 |
| ATOM | 1793 | CA | ASN | 1 | 30 | 22.612 | 48.501 | 8.965 | 1.00 | 0.00 |
| ATOM | 1794 | C | ASN | 1 | 30 | 22.217 | 48.513 | 10.413 | 1.00 | 0.00 |
| ATOM | 1795 | O | ASN | 1 | 30 | 22.389 | 49.532 | 11.082 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1796 | CB | ASN | 1 | 30 | 21.422 | 48.940 | 8.120 | 1.00 | 0.00 |
| ATOM | 1797 | CG | ASN | 1 | 30 | 21.971 | 49.646 | 6.912 | 1.00 | 0.00 |
| ATOM | 1798 | OD1 | ASN | 1 | 30 | 22.845 | 50.501 | 7.008 | 1.00 | 0.00 |
| ATOM | 1799 | ND2 | ASN | 1 | 30 | 21.484 | 49.202 | 5.763 | 1.00 | 0.00 |
| ATOM | 1800 | H | ASN | 1 | 30 | 22.675 | 46.431 | 8.312 | 1.00 | 0.00 |
| ATOM | 1801 | 1HD2 | ASN | 1 | 30 | 21.820 | 49.588 | 4.905 | 1.00 | 0.00 |
| ATOM | 1802 | 2HD2 | ASN | 1 | 30 | 20.779 | 48.494 | 5.712 | 1.00 | 0.00 |
| ATOM | 1803 | N | GLU | 1 | 31 | 21.711 | 47.348 | 10.868 | 1.00 | 0.00 |
| ATOM | 1804 | CA | GLU | 1 | 31 | 21.351 | 47.068 | 12.262 | 1.00 | 0.00 |
| ATOM | 1805 | C | GLU | 1 | 31 | 21.898 | 48.089 | 13.237 | 1.00 | 0.00 |
| ATOM | 1806 | O | GLU | 1 | 31 | 23.100 | 48.202 | 13.412 | 1.00 | 0.00 |
| ATOM | 1807 | CB | GLU | 1 | 31 | 21.817 | 45.651 | 12.620 | 1.00 | 0.00 |
| ATOM | 1808 | CG | GLU | 1 | 31 | 21.110 | 44.977 | 13.804 | 1.00 | 0.00 |
| ATOM | 1809 | CD | GLU | 1 | 31 | 21.335 | 45.730 | 15.099 | 1.00 | 0.00 |
| ATOM | 1810 | OE1 | GLU | 1 | 31 | 22.269 | 45.422 | 15.820 | 1.00 | 0.00 |
| ATOM | 1811 | OE2 | GLU | 1 | 31 | 20.593 | 46.652 | 15.418 | 1.00 | 0.00 |
| ATOM | 1812 | H | GLU | 1 | 31 | 21.520 | 46.627 | 10.201 | 1.00 | 0.00 |
| ATOM | 1813 | N | ARG | 1 | 32 | 21.017 | 48.924 | 13.805 | 1.00 | 0.00 |
| ATOM | 1814 | CA | ARG | 1 | 32 | 21.534 | 50.184 | 14.222 | 1.00 | 0.00 |
| ATOM | 1815 | C | ARG | 1 | 32 | 22.729 | 50.149 | 15.274 | 1.00 | 0.00 |
| ATOM | 1816 | O | ARG | 1 | 32 | 22.607 | 49.779 | 16.436 | 1.00 | 0.00 |
| ATOM | 1817 | CB | ARG | 1 | 32 | 20.634 | 51.305 | 14.473 | 1.00 | 0.00 |
| ATOM | 1818 | CG | ARG | 1 | 32 | 20.856 | 52.397 | 13.422 | 1.00 | 0.00 |
| ATOM | 1819 | CD | ARG | 1 | 32 | 20.843 | 53.815 | 13.995 | 1.00 | 0.00 |
| ATOM | 1820 | NE | ARG | 1 | 32 | 21.877 | 53.966 | 15.017 | 1.00 | 0.00 |
| ATOM | 1821 | CZ | ARG | 1 | 32 | 21.557 | 54.361 | 16.270 | 1.00 | 0.00 |
| ATOM | 1822 | NH1 | ARG | 1 | 32 | 22.511 | 54.352 | 17.188 | 1.00 | 0.00 |
| ATOM | 1823 | NH2 | ARG | 1 | 32 | 20.314 | 54.719 | 16.578 | 1.00 | 0.00 |
| ATOM | 1824 | H | ARG | 1 | 32 | 20.112 | 48.610 | 14.084 | 1.00 | 0.00 |
| ATOM | 1825 | HE | ARG | 1 | 32 | 22.829 | 53.699 | 14.846 | 1.00 | 0.00 |
| ATOM | 1826 | 1HH1 | ARG | 1 | 32 | 23.435 | 54.026 | 16.968 | 1.00 | 0.00 |
| ATOM | 1827 | 2HH1 | ARG | 1 | 32 | 22.330 | 54.615 | 18.133 | 1.00 | 0.00 |
| ATOM | 1828 | 1HH2 | ARG | 1 | 32 | 20.085 | 54.891 | 17.541 | 1.00 | 0.00 |
| ATOM | 1829 | 2HH2 | ARG | 1 | 32 | 19.607 | 54.849 | 15.989 | 1.00 | 0.00 |
| ATOM | 1830 | N | TYR | 1 | 33 | 23.699 | 50.538 | 14.784 | 1.00 | 0.00 |
| ATOM | 1831 | CA | TYR | 1 | 33 | 25.025 | 50.585 | 15.715 | 1.00 | 0.00 |
| ATOM | 1832 | C | TYR | 1 | 33 | 25.194 | 52.007 | 16.204 | 1.00 | 0.00 |
| ATOM | 1833 | O | TYR | 1 | 33 | 24.355 | 52.825 | 15.804 | 1.00 | 0.00 |
| ATOM | 1834 | CB | TYR | 1 | 33 | 26.228 | 49.919 | 15.047 | 1.00 | 0.00 |
| ATOM | 1835 | CG | TYR | 1 | 33 | 25.888 | 48.462 | 14.763 | 1.00 | 0.00 |
| ATOM | 1836 | CD1 | TYR | 1 | 33 | 25.902 | 47.980 | 13.434 | 1.00 | 0.00 |
| ATOM | 1837 | CD2 | TYR | 1 | 33 | 25.568 | 47.615 | 15.845 | 1.00 | 0.00 |
| ATOM | 1838 | CE1 | TYR | 1 | 33 | 25.641 | 46.613 | 13.192 | 1.00 | 0.00 |
| ATOM | 1839 | CE2 | TYR | 1 | 33 | 25.314 | 46.255 | 15.504 | 1.00 | 0.00 |
| ATOM | 1840 | CZ | TYR | 1 | 33 | 25.387 | 45.757 | 14.287 | 1.00 | 0.00 |
| ATOM | 1841 | OH | TYR | 1 | 33 | 25.239 | 44.392 | 14.090 | 1.00 | 0.00 |
| ATOM | 1842 | H | TYR | 1 | 33 | 23.974 | 50.778 | 13.814 | 1.00 | 0.00 |
| ATOM | 1843 | HH | TYR | 1 | 33 | 25.245 | 44.015 | 14.970 | 1.00 | 0.00 |
| ATOM | 1844 | N | GLU | 1 | 34 | 26.194 | 52.266 | 17.080 | 1.00 | 0.00 |
| ATOM | 1845 | CA | GLU | 1 | 34 | 26.183 | 53.569 | 17.764 | 1.00 | 0.00 |
| ATOM | 1846 | C | GLU | 1 | 34 | 26.105 | 54.817 | 16.890 | 1.00 | 0.00 |
| ATOM | 1847 | O | GLU | 1 | 34 | 26.239 | 54.806 | 15.665 | 1.00 | 0.00 |
| ATOM | 1848 | CB | GLU | 1 | 34 | 27.215 | 53.643 | 18.919 | 1.00 | 0.00 |
| ATOM | 1849 | CG | GLU | 1 | 34 | 28.684 | 54.047 | 18.684 | 1.00 | 0.00 |
| ATOM | 1850 | CD | GLU | 1 | 34 | 28.956 | 55.514 | 19.011 | 1.00 | 0.00 |
| ATOM | 1851 | OE1 | GLU | 1 | 34 | 28.301 | 56.386 | 18.474 | 1.00 | 0.00 |
| ATOM | 1852 | OE2 | GLU | 1 | 34 | 29.849 | 55.831 | 19.790 | 1.00 | 0.00 |
| ATOM | 1853 | H | GLU | 1 | 34 | 26.823 | 51.551 | 17.373 | 1.00 | 0.00 |
| ATOM | 1854 | N | GLY | 1 | 35 | 25.729 | 55.900 | 17.584 | 1.00 | 0.00 |
| ATOM | 1855 | CA | GLY | 1 | 35 | 25.444 | 57.105 | 16.825 | 1.00 | 0.00 |
| ATOM | 1856 | C | GLY | 1 | 35 | 26.703 | 57.810 | 16.386 | 1.00 | 0.00 |
| ATOM | 1857 | O | GLY | 1 | 35 | 27.285 | 57.509 | 15.343 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1858 | H | GLY | 1 | 35 | 26.095 | 55.942 | 18.517 | 1.00 | 0.00 |
| ATOM | 1859 | N | TYR | 1 | 36 | 27.090 | 58.770 | 17.226 | 1.00 | 0.00 |
| ATOM | 1860 | CA | TYR | 1 | 36 | 28.194 | 59.639 | 16.834 | 1.00 | 0.00 |
| ATOM | 1861 | C | TYR | 1 | 36 | 29.509 | 58.939 | 16.496 | 1.00 | 0.00 |
| ATOM | 1862 | O | TYR | 1 | 36 | 30.058 | 59.071 | 15.413 | 1.00 | 0.00 |
| ATOM | 1863 | CB | TYR | 1 | 36 | 28.366 | 60.742 | 17.891 | 1.00 | 0.00 |
| ATOM | 1864 | CG | TYR | 1 | 36 | 29.555 | 61.623 | 17.582 | 1.00 | 0.00 |
| ATOM | 1865 | CD1 | TYR | 1 | 36 | 30.353 | 62.051 | 18.658 | 1.00 | 0.00 |
| ATOM | 1866 | CD2 | TYR | 1 | 36 | 29.858 | 61.955 | 16.243 | 1.00 | 0.00 |
| ATOM | 1867 | CE1 | TYR | 1 | 36 | 31.525 | 62.764 | 18.378 | 1.00 | 0.00 |
| ATOM | 1868 | CE2 | TYR | 1 | 36 | 31.046 | 62.630 | 15.963 | 1.00 | 0.00 |
| ATOM | 1869 | CZ | TYR | 1 | 36 | 31.866 | 63.014 | 17.035 | 1.00 | 0.00 |
| ATOM | 1870 | OH | TYR | 1 | 36 | 33.045 | 63.668 | 16.753 | 1.00 | 0.00 |
| ATOM | 1871 | H | TYR | 1 | 36 | 26.758 | 58.690 | 18.164 | 1.00 | 0.00 |
| ATOM | 1872 | HH | TYR | 1 | 36 | 33.412 | 63.310 | 15.941 | 1.00 | 0.00 |
| ATOM | 1873 | N | CYS | 1 | 37 | 30.018 | 58.198 | 17.474 | 1.00 | 0.00 |
| ATOM | 1874 | CA | CYS | 1 | 37 | 31.238 | 57.457 | 17.157 | 1.00 | 0.00 |
| ATOM | 1875 | C | CYS | 1 | 37 | 31.062 | 56.100 | 16.484 | 1.00 | 0.00 |
| ATOM | 1876 | O | CYS | 1 | 37 | 31.981 | 55.294 | 16.349 | 1.00 | 0.00 |
| ATOM | 1877 | CB | CYS | 1 | 37 | 32.156 | 57.390 | 18.373 | 1.00 | 0.00 |
| ATOM | 1878 | SG | CYS | 1 | 37 | 32.395 | 59.035 | 19.101 | 1.00 | 0.00 |
| ATOM | 1879 | H | CYS | 1 | 37 | 29.514 | 58.042 | 18.328 | 1.00 | 0.00 |
| ATOM | 1880 | N | VAL | 1 | 38 | 29.846 | 55.866 | 15.969 | 1.00 | 0.00 |
| ATOM | 1881 | CA | VAL | 1 | 38 | 29.923 | 54.999 | 14.798 | 1.00 | 0.00 |
| ATOM | 1882 | C | VAL | 1 | 38 | 30.145 | 55.768 | 13.514 | 1.00 | 0.00 |
| ATOM | 1883 | O | VAL | 1 | 38 | 30.839 | 55.302 | 12.620 | 1.00 | 0.00 |
| ATOM | 1884 | CB | VAL | 1 | 38 | 28.803 | 53.949 | 14.723 | 1.00 | 0.00 |
| ATOM | 1885 | CG1 | VAL | 1 | 38 | 28.244 | 53.637 | 13.328 | 1.00 | 0.00 |
| ATOM | 1886 | CG2 | VAL | 1 | 38 | 29.294 | 52.682 | 15.417 | 1.00 | 0.00 |
| ATOM | 1887 | H | VAL | 1 | 38 | 29.033 | 56.367 | 16.253 | 1.00 | 0.00 |
| ATOM | 1888 | N | ASP | 1 | 39 | 29.622 | 57.002 | 13.458 | 1.00 | 0.00 |
| ATOM | 1889 | CA | ASP | 1 | 39 | 29.863 | 57.865 | 12.288 | 1.00 | 0.00 |
| ATOM | 1890 | C | ASP | 1 | 39 | 31.322 | 58.314 | 12.168 | 1.00 | 0.00 |
| ATOM | 1891 | O | ASP | 1 | 39 | 31.989 | 58.296 | 11.129 | 1.00 | 0.00 |
| ATOM | 1892 | CB | ASP | 1 | 39 | 28.802 | 58.936 | 12.308 | 1.00 | 0.00 |
| ATOM | 1893 | CG | ASP | 1 | 39 | 29.307 | 60.403 | 12.000 | 1.00 | 0.00 |
| ATOM | 1894 | OD1 | ASP | 1 | 39 | 28.990 | 60.956 | 10.958 | 1.00 | 0.00 |
| ATOM | 1895 | OD2 | ASP | 1 | 39 | 29.999 | 60.989 | 12.818 | 1.00 | 0.00 |
| ATOM | 1896 | H | ASP | 1 | 39 | 29.100 | 57.372 | 14.226 | 1.00 | 0.00 |
| ATOM | 1897 | N | LEU | 1 | 40 | 31.857 | 58.672 | 13.353 | 1.00 | 0.00 |
| ATOM | 1898 | CA | LEU | 1 | 40 | 33.304 | 58.811 | 13.510 | 1.00 | 0.00 |
| ATOM | 1899 | C | LEU | 1 | 40 | 34.024 | 57.573 | 13.012 | 1.00 | 0.00 |
| ATOM | 1900 | O | LEU | 1 | 40 | 34.779 | 57.643 | 12.044 | 1.00 | 0.00 |
| ATOM | 1901 | CB | LEU | 1 | 40 | 33.673 | 59.157 | 14.958 | 1.00 | 0.00 |
| ATOM | 1902 | CG | LEU | 1 | 40 | 35.175 | 59.350 | 15.204 | 1.00 | 0.00 |
| ATOM | 1903 | CD1 | LEU | 1 | 40 | 35.773 | 60.492 | 14.381 | 1.00 | 0.00 |
| ATOM | 1904 | CD2 | LEU | 1 | 40 | 35.490 | 59.492 | 16.692 | 1.00 | 0.00 |
| ATOM | 1905 | H | LEU | 1 | 40 | 31.190 | 58.816 | 14.080 | 1.00 | 0.00 |
| ATOM | 1906 | N | ALA | 1 | 41 | 33.673 | 56.444 | 13.648 | 1.00 | 0.00 |
| ATOM | 1907 | CA | ALA | 1 | 41 | 34.130 | 55.160 | 13.129 | 1.00 | 0.00 |
| ATOM | 1908 | C | ALA | 1 | 41 | 33.970 | 54.920 | 11.638 | 1.00 | 0.00 |
| ATOM | 1909 | O | ALA | 1 | 41 | 34.778 | 54.197 | 11.075 | 1.00 | 0.00 |
| ATOM | 1910 | CB | ALA | 1 | 41 | 33.475 | 53.993 | 13.860 | 1.00 | 0.00 |
| ATOM | 1911 | H | ALA | 1 | 41 | 33.128 | 56.510 | 14.487 | 1.00 | 0.00 |
| ATOM | 1912 | N | VAL | 1 | 42 | 32.964 | 55.541 | 11.000 | 1.00 | 0.00 |
| ATOM | 1913 | CA | VAL | 1 | 42 | 32.879 | 55.340 | 9.550 | 1.00 | 0.00 |
| ATOM | 1914 | C | VAL | 1 | 42 | 34.136 | 55.808 | 8.832 | 1.00 | 0.00 |
| ATOM | 1915 | O | VAL | 1 | 42 | 34.684 | 55.126 | 7.966 | 1.00 | 0.00 |
| ATOM | 1916 | CB | VAL | 1 | 42 | 31.605 | 55.965 | 8.947 | 1.00 | 0.00 |
| ATOM | 1917 | CG1 | VAL | 1 | 42 | 31.567 | 55.904 | 7.415 | 1.00 | 0.00 |
| ATOM | 1918 | CG2 | VAL | 1 | 42 | 30.361 | 55.286 | 9.520 | 1.00 | 0.00 |
| ATOM | 1919 | H | VAL | 1 | 42 | 32.370 | 56.179 | 11.493 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1920 | N | GLU | 1 | 43 | 34.629 | 56.974 | 9.260 | 1.00 | 0.00 |
| ATOM | 1921 | CA | GLU | 1 | 43 | 35.939 | 57.298 | 8.714 | 1.00 | 0.00 |
| ATOM | 1922 | C | GLU | 1 | 43 | 37.165 | 56.694 | 9.389 | 1.00 | 0.00 |
| ATOM | 1923 | O | GLU | 1 | 43 | 38.229 | 56.677 | 8.792 | 1.00 | 0.00 |
| ATOM | 1924 | CB | GLU | 1 | 43 | 36.102 | 58.796 | 8.412 | 1.00 | 0.00 |
| ATOM | 1925 | CG | GLU | 1 | 43 | 35.403 | 59.272 | 7.115 | 1.00 | 0.00 |
| ATOM | 1926 | CD | GLU | 1 | 43 | 36.041 | 58.739 | 5.824 | 1.00 | 0.00 |
| ATOM | 1927 | OE1 | GLU | 1 | 43 | 36.893 | 57.861 | 5.864 | 1.00 | 0.00 |
| ATOM | 1928 | OE2 | GLU | 1 | 43 | 35.692 | 59.180 | 4.729 | 1.00 | 0.00 |
| ATOM | 1929 | H | GLU | 1 | 43 | 34.088 | 57.569 | 9.856 | 1.00 | 0.00 |
| ATOM | 1930 | N | ILE | 1 | 44 | 37.042 | 56.147 | 10.603 | 1.00 | 0.00 |
| ATOM | 1931 | CA | ILE | 1 | 44 | 38.247 | 55.435 | 11.069 | 1.00 | 0.00 |
| ATOM | 1932 | C | ILE | 1 | 44 | 38.433 | 54.102 | 10.332 | 1.00 | 0.00 |
| ATOM | 1933 | O | ILE | 1 | 44 | 39.487 | 53.733 | 9.799 | 1.00 | 0.00 |
| ATOM | 1934 | CB | ILE | 1 | 44 | 38.284 | 55.291 | 12.598 | 1.00 | 0.00 |
| ATOM | 1935 | CG1 | ILE | 1 | 44 | 37.781 | 56.572 | 13.270 | 1.00 | 0.00 |
| ATOM | 1936 | CG2 | ILE | 1 | 44 | 39.721 | 55.007 | 13.049 | 1.00 | 0.00 |
| ATOM | 1937 | CD1 | ILE | 1 | 44 | 37.685 | 56.440 | 14.789 | 1.00 | 0.00 |
| ATOM | 1938 | H | ILE | 1 | 44 | 36.177 | 56.236 | 11.100 | 1.00 | 0.00 |
| ATOM | 1939 | N | ALA | 1 | 45 | 37.264 | 53.481 | 10.164 | 1.00 | 0.00 |
| ATOM | 1940 | CA | ALA | 1 | 45 | 37.118 | 52.429 | 9.168 | 1.00 | 0.00 |
| ATOM | 1941 | C | ALA | 1 | 45 | 37.696 | 52.838 | 7.826 | 1.00 | 0.00 |
| ATOM | 1942 | O | ALA | 1 | 45 | 38.604 | 52.198 | 7.304 | 1.00 | 0.00 |
| ATOM | 1943 | CB | ALA | 1 | 45 | 35.649 | 52.038 | 8.993 | 1.00 | 0.00 |
| ATOM | 1944 | H | ALA | 1 | 45 | 36.568 | 53.672 | 10.352 | 1.00 | 0.00 |
| ATOM | 1945 | N | LYS | 1 | 46 | 37.179 | 53.954 | 7.307 | 1.00 | 0.00 |
| ATOM | 1946 | CA | LYS | 1 | 46 | 37.516 | 54.307 | 5.928 | 1.00 | 0.00 |
| ATOM | 1947 | C | LYS | 1 | 46 | 38.627 | 55.335 | 5.672 | 1.00 | 0.00 |
| ATOM | 1948 | O | LYS | 1 | 46 | 38.754 | 55.906 | 4.579 | 1.00 | 0.00 |
| ATOM | 1949 | CB | LYS | 1 | 46 | 36.227 | 54.658 | 5.184 | 1.00 | 0.00 |
| ATOM | 1950 | CG | LYS | 1 | 46 | 36.207 | 54.291 | 3.696 | 1.00 | 0.00 |
| ATOM | 1951 | CD | LYS | 1 | 46 | 36.261 | 55.197 | 2.901 | 1.00 | 0.00 |
| ATOM | 1952 | CE | LYS | 1 | 46 | 35.899 | 56.499 | 2.384 | 1.00 | 0.00 |
| ATOM | 1953 | NZ | LYS | 1 | 46 | 36.640 | 57.192 | 3.437 | 1.00 | 0.00 |
| ATOM | 1954 | H | LYS | 1 | 46 | 36.474 | 54.440 | 7.826 | 1.00 | 0.00 |
| ATOM | 1955 | 1HZ | LYS | 1 | 46 | 36.744 | 58.213 | 3.291 | 1.00 | 0.00 |
| ATOM | 1956 | 2HZ | LYS | 1 | 46 | 36.128 | 57.187 | 4.346 | 1.00 | 0.00 |
| ATOM | 1957 | 3HZ | LYS | 1 | 46 | 37.561 | 56.753 | 3.635 | 1.00 | 0.00 |
| ATOM | 1958 | N | MET | 1 | 47 | 39.475 | 55.534 | 6.698 | 1.00 | 0.00 |
| ATOM | 1959 | CA | MET | 1 | 47 | 40.732 | 56.229 | 6.410 | 1.00 | 0.00 |
| ATOM | 1960 | C | MET | 1 | 47 | 41.779 | 55.208 | 6.009 | 1.00 | 0.00 |
| ATOM | 1961 | O | MET | 1 | 47 | 42.510 | 55.330 | 5.027 | 1.00 | 0.00 |
| ATOM | 1962 | CB | MET | 1 | 47 | 41.193 | 57.061 | 7.611 | 1.00 | 0.00 |
| ATOM | 1963 | CG | MET | 1 | 47 | 42.325 | 58.040 | 7.284 | 1.00 | 0.00 |
| ATOM | 1964 | SD | MET | 1 | 47 | 42.856 | 58.984 | 8.721 | 1.00 | 0.00 |
| ATOM | 1965 | CE | MET | 1 | 47 | 43.993 | 60.110 | 7.898 | 1.00 | 0.00 |
| ATOM | 1966 | H | MET | 1 | 47 | 39.207 | 55.338 | 7.642 | 1.00 | 0.00 |
| ATOM | 1967 | N | VAL | 1 | 48 | 41.724 | 54.125 | 6.808 | 1.00 | 0.00 |
| ATOM | 1968 | CA | VAL | 1 | 48 | 42.380 | 52.861 | 6.469 | 1.00 | 0.00 |
| ATOM | 1969 | C | VAL | 1 | 48 | 41.741 | 52.170 | 5.264 | 1.00 | 0.00 |
| ATOM | 1970 | O | VAL | 1 | 48 | 42.405 | 51.585 | 4.417 | 1.00 | 0.00 |
| ATOM | 1971 | CB | VAL | 1 | 48 | 42.368 | 51.937 | 7.702 | 1.00 | 0.00 |
| ATOM | 1972 | CG1 | VAL | 1 | 48 | 43.102 | 50.614 | 7.458 | 1.00 | 0.00 |
| ATOM | 1973 | CG2 | VAL | 1 | 48 | 42.920 | 52.657 | 8.936 | 1.00 | 0.00 |
| ATOM | 1974 | H | VAL | 1 | 48 | 41.192 | 54.228 | 7.652 | 1.00 | 0.00 |
| ATOM | 1975 | N | ARG | 1 | 49 | 40.401 | 52.285 | 5.226 | 1.00 | 0.00 |
| ATOM | 1976 | CA | ARG | 1 | 49 | 39.515 | 51.624 | 4.250 | 1.00 | 0.00 |
| ATOM | 1977 | C | ARG | 1 | 49 | 39.246 | 50.155 | 4.532 | 1.00 | 0.00 |
| ATOM | 1978 | O | ARG | 1 | 49 | 39.057 | 49.314 | 3.658 | 1.00 | 0.00 |
| ATOM | 1979 | CB | ARG | 1 | 49 | 39.860 | 51.820 | 2.762 | 1.00 | 0.00 |
| ATOM | 1980 | CG | ARG | 1 | 49 | 39.836 | 53.257 | 2.229 | 1.00 | 0.00 |
| ATOM | 1981 | CD | ARG | 1 | 49 | 41.190 | 53.961 | 2.324 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1982 | NE | ARG | 1 | 49 | 42.210 | 53.192 | 1.610 | 1.00 | 0.00 |
| ATOM | 1983 | CZ | ARG | 1 | 49 | 43.511 | 53.272 | 1.955 | 1.00 | 0.00 |
| ATOM | 1984 | NH1 | ARG | 1 | 49 | 44.408 | 52.590 | 1.248 | 1.00 | 0.00 |
| ATOM | 1985 | NH2 | ARG | 1 | 49 | 43.897 | 54.033 | 2.978 | 1.00 | 0.00 |
| ATOM | 1986 | H | ARG | 1 | 49 | 40.006 | 52.729 | 6.031 | 1.00 | 0.00 |
| ATOM | 1987 | HE | ARG | 1 | 49 | 41.909 | 52.589 | 0.870 | 1.00 | 0.00 |
| ATOM | 1988 | 1HH1 | ARG | 1 | 49 | 45.385 | 52.656 | 1.440 | 1.00 | 0.00 |
| ATOM | 1989 | 2HH1 | ARG | 1 | 49 | 44.104 | 51.984 | 0.513 | 1.00 | 0.00 |
| ATOM | 1990 | 1HH2 | ARG | 1 | 49 | 44.856 | 54.196 | 3.201 | 1.00 | 0.00 |
| ATOM | 1991 | 2HH2 | ARG | 1 | 49 | 43.205 | 54.453 | 3.578 | 1.00 | 0.00 |
| ATOM | 1992 | N | ILE | 1 | 50 | 39.206 | 49.881 | 5.835 | 1.00 | 0.00 |
| ATOM | 1993 | CA | ILE | 1 | 50 | 38.465 | 48.676 | 6.201 | 1.00 | 0.00 |
| ATOM | 1994 | C | ILE | 1 | 50 | 37.031 | 49.128 | 6.464 | 1.00 | 0.00 |
| ATOM | 1995 | O | ILE | 1 | 50 | 36.792 | 50.325 | 6.603 | 1.00 | 0.00 |
| ATOM | 1996 | CB | ILE | 1 | 50 | 39.156 | 48.013 | 7.414 | 1.00 | 0.00 |
| ATOM | 1997 | CG1 | ILE | 1 | 50 | 38.600 | 46.529 | 7.775 | 1.00 | 0.00 |
| ATOM | 1998 | CG2 | ILE | 1 | 50 | 39.154 | 48.952 | 8.629 | 1.00 | 0.00 |
| ATOM | 1999 | CD1 | ILE | 1 | 50 | 39.392 | 45.929 | 8.882 | 1.00 | 0.00 |
| ATOM | 2000 | H | ILE | 1 | 50 | 39.353 | 50.605 | 6.508 | 1.00 | 0.00 |
| ATOM | 2001 | N | LYS | 1 | 51 | 36.079 | 48.194 | 6.530 | 1.00 | 0.00 |
| ATOM | 2002 | CA | LYS | 1 | 51 | 34.892 | 48.605 | 7.265 | 1.00 | 0.00 |
| ATOM | 2003 | C | LYS | 1 | 51 | 34.707 | 47.725 | 8.477 | 1.00 | 0.00 |
| ATOM | 2004 | O | LYS | 1 | 51 | 34.801 | 46.495 | 8.429 | 1.00 | 0.00 |
| ATOM | 2005 | CB | LYS | 1 | 51 | 33.639 | 48.722 | 6.381 | 1.00 | 0.00 |
| ATOM | 2006 | CG | LYS | 1 | 51 | 32.586 | 49.643 | 7.022 | 1.00 | 0.00 |
| ATOM | 2007 | CD | LYS | 1 | 51 | 31.441 | 50.067 | 6.093 | 1.00 | 0.00 |
| ATOM | 2008 | CE | LYS | 1 | 51 | 30.449 | 51.017 | 6.782 | 1.00 | 0.00 |
| ATOM | 2009 | NZ | LYS | 1 | 51 | 29.443 | 51.501 | 5.821 | 1.00 | 0.00 |
| ATOM | 2010 | H | LYS | 1 | 51 | 36.198 | 47.246 | 6.242 | 1.00 | 0.00 |
| ATOM | 2011 | 1HZ | LYS | 1 | 51 | 29.894 | 52.123 | 5.122 | 1.00 | 0.00 |
| ATOM | 2012 | 2HZ | LYS | 1 | 51 | 28.989 | 50.724 | 5.307 | 1.00 | 0.00 |
| ATOM | 2013 | 3HZ | LYS | 1 | 51 | 28.687 | 52.022 | 6.308 | 1.00 | 0.00 |
| ATOM | 2014 | N | TYR | 1 | 52 | 34.526 | 48.431 | 9.597 | 1.00 | 0.00 |
| ATOM | 2015 | CA | TYR | 1 | 52 | 34.487 | 47.731 | 10.875 | 1.00 | 0.00 |
| ATOM | 2016 | C | TYR | 1 | 52 | 33.276 | 46.843 | 10.982 | 1.00 | 0.00 |
| ATOM | 2017 | O | TYR | 1 | 52 | 32.355 | 46.909 | 10.166 | 1.00 | 0.00 |
| ATOM | 2018 | CB | TYR | 1 | 52 | 34.473 | 48.721 | 12.040 | 1.00 | 0.00 |
| ATOM | 2019 | CG | TYR | 1 | 52 | 35.713 | 49.584 | 12.113 | 1.00 | 0.00 |
| ATOM | 2020 | CD1 | TYR | 1 | 52 | 35.554 | 50.920 | 12.529 | 1.00 | 0.00 |
| ATOM | 2021 | CD2 | TYR | 1 | 52 | 36.981 | 49.047 | 11.807 | 1.00 | 0.00 |
| ATOM | 2022 | CE1 | TYR | 1 | 52 | 36.686 | 51.728 | 12.701 | 1.00 | 0.00 |
| ATOM | 2023 | CE2 | TYR | 1 | 52 | 38.112 | 49.866 | 11.940 | 1.00 | 0.00 |
| ATOM | 2024 | CZ | TYR | 1 | 52 | 37.946 | 51.190 | 12.389 | 1.00 | 0.00 |
| ATOM | 2025 | OH | TYR | 1 | 52 | 39.072 | 51.978 | 12.502 | 1.00 | 0.00 |
| ATOM | 2026 | H | TYR | 1 | 52 | 34.414 | 49.426 | 9.592 | 1.00 | 0.00 |
| ATOM | 2027 | HH | TYR | 1 | 52 | 38.902 | 62.637 | 13.179 | 1.00 | 0.00 |
| ATOM | 2028 | N | LYS | 1 | 53 | 33.292 | 45.988 | 12.103 | 1.00 | 0.00 |
| ATOM | 2029 | CA | LYS | 1 | 53 | 32.001 | 45.475 | 12.449 | 1.00 | 0.00 |
| ATOM | 2030 | C | LYS | 1 | 53 | 31.554 | 46.385 | 13.569 | 1.00 | 0.00 |
| ATOM | 2031 | O | LYS | 1 | 53 | 31.864 | 46.178 | 14.736 | 1.00 | 0.00 |
| ATOM | 2032 | CB | LYS | 1 | 53 | 32.095 | 44.015 | 12.907 | 1.00 | 0.00 |
| ATOM | 2033 | CG | LYS | 1 | 53 | 30.736 | 43.331 | 13.115 | 1.00 | 0.00 |
| ATOM | 2034 | CD | LYS | 1 | 53 | 30.842 | 42.007 | 13.884 | 1.00 | 0.00 |
| ATOM | 2035 | CE | LYS | 1 | 53 | 29.518 | 41.239 | 14.029 | 1.00 | 0.00 |
| ATOM | 2036 | NZ | LYS | 1 | 53 | 29.193 | 40.557 | 12.770 | 1.00 | 0.00 |
| ATOM | 2037 | H | LYS | 1 | 53 | 34.047 | 45.978 | 12.670 | 1.00 | 0.00 |
| ATOM | 2038 | 1HZ | LYS | 1 | 53 | 29.093 | 41.231 | 11.977 | 1.00 | 0.00 |
| ATOM | 2039 | 2HZ | LYS | 1 | 53 | 29.871 | 39.827 | 12.494 | 1.00 | 0.00 |
| ATOM | 2040 | 3HZ | LYS | 1 | 53 | 28.245 | 40.125 | 12.772 | 1.00 | 0.00 |
| ATOM | 2041 | N | LEU | 1 | 54 | 30.878 | 47.455 | 13.134 | 1.00 | 0.00 |
| ATOM | 2042 | CA | LEU | 1 | 54 | 30.228 | 48.286 | 14.140 | 1.00 | 0.00 |
| ATOM | 2043 | C | LEU | 1 | 54 | 29.186 | 47.391 | 14.779 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2044 | O | LEU | 1 | 54 | 28.393 | 46.816 | 14.033 | 1.00 | 0.00 |
| ATOM | 2045 | CB | LEU | 1 | 54 | 29.548 | 49.456 | 13.424 | 1.00 | 0.00 |
| ATOM | 2046 | CG | LEU | 1 | 54 | 30.342 | 50.057 | 12.255 | 1.00 | 0.00 |
| ATOM | 2047 | CD1 | LEU | 1 | 54 | 29.424 | 50.707 | 11.219 | 1.00 | 0.00 |
| ATOM | 2048 | CD2 | LEU | 1 | 54 | 31.451 | 51.002 | 12.709 | 1.00 | 0.00 |
| ATOM | 2049 | H | LEU | 1 | 54 | 30.575 | 47.461 | 12.186 | 1.00 | 0.00 |
| ATOM | 2050 | N | SER | 1 | 55 | 29.251 | 47.248 | 16.102 | 1.00 | 0.00 |
| ATOM | 2051 | CA | SER | 1 | 55 | 28.540 | 46.131 | 16.711 | 1.00 | 0.00 |
| ATOM | 2052 | C | SER | 1 | 55 | 28.364 | 46.313 | 18.196 | 1.00 | 0.00 |
| ATOM | 2053 | O | SER | 1 | 55 | 29.096 | 47.015 | 18.895 | 1.00 | 0.00 |
| ATOM | 2054 | CB | SER | 1 | 55 | 29.233 | 44.784 | 16.435 | 1.00 | 0.00 |
| ATOM | 2055 | OG | SER | 1 | 55 | 28.325 | 43.633 | 16.602 | 1.00 | 0.00 |
| ATOM | 2056 | H | SER | 1 | 55 | 29.960 | 47.724 | 16.622 | 1.00 | 0.00 |
| ATOM | 2057 | HG | SER | 1 | 55 | 28.560 | 43.291 | 17.457 | 1.00 | 0.00 |
| ATOM | 2058 | N | ILE | 1 | 56 | 27.342 | 45.610 | 18.663 | 1.00 | 0.00 |
| ATOM | 2059 | CA | ILE | 1 | 56 | 27.296 | 45.299 | 20.073 | 1.00 | 0.00 |
| ATOM | 2060 | C | ILE | 1 | 56 | 27.607 | 43.811 | 20.153 | 1.00 | 0.00 |
| ATOM | 2061 | O | ILE | 1 | 56 | 27.284 | 43.050 | 19.236 | 1.00 | 0.00 |
| ATOM | 2062 | CB | ILE | 1 | 56 | 25.905 | 45.708 | 20.609 | 1.00 | 0.00 |
| ATOM | 2063 | CG1 | ILE | 1 | 56 | 25.756 | 45.571 | 22.122 | 1.00 | 0.00 |
| ATOM | 2064 | CG2 | ILE | 1 | 56 | 24.772 | 44.974 | 19.874 | 1.00 | 0.00 |
| ATOM | 2065 | CD1 | ILE | 1 | 56 | 24.492 | 46.238 | 22.668 | 1.00 | 0.00 |
| ATOM | 2066 | H | ILE | 1 | 56 | 26.750 | 45.100 | 18.038 | 1.00 | 0.00 |
| ATOM | 2067 | N | VAL | 1 | 57 | 28.296 | 43.397 | 21.216 | 1.00 | 0.00 |
| ATOM | 2068 | CA | VAL | 1 | 57 | 28.397 | 41.947 | 21.398 | 1.00 | 0.00 |
| ATOM | 2069 | C | VAL | 1 | 57 | 27.314 | 41.502 | 22.274 | 1.00 | 0.00 |
| ATOM | 2070 | O | VAL | 1 | 57 | 26.175 | 41.226 | 21.995 | 1.00 | 0.00 |
| ATOM | 2071 | CB | VAL | 1 | 57 | 29.836 | 41.509 | 21.756 | 1.00 | 0.00 |
| ATOM | 2072 | CG1 | VAL | 1 | 57 | 30.623 | 41.264 | 20.467 | 1.00 | 0.00 |
| ATOM | 2073 | CG2 | VAL | 1 | 57 | 30.588 | 42.485 | 22.676 | 1.00 | 0.00 |
| ATOM | 2074 | H | VAL | 1 | 57 | 28.537 | 44.072 | 21.920 | 1.00 | 0.00 |
| ATOM | 2075 | N | GLY | 1 | 58 | 27.672 | 41.580 | 23.667 | 1.00 | 0.00 |
| ATOM | 2076 | CA | GLY | 1 | 58 | 26.771 | 42.256 | 24.596 | 1.00 | 0.00 |
| ATOM | 2077 | C | GLY | 1 | 58 | 27.313 | 42.651 | 24.867 | 1.00 | 0.00 |
| ATOM | 2078 | O | GLY | 1 | 58 | 27.892 | 44.257 | 23.974 | 1.00 | 0.00 |
| ATOM | 2079 | H | GLY | 1 | 58 | 28.633 | 41.462 | 23.908 | 1.00 | 0.00 |
| ATOM | 2080 | N | ASP | 1 | 59 | 27.118 | 44.099 | 26.117 | 1.00 | 0.00 |
| ATOM | 2081 | CA | ASP | 1 | 59 | 27.586 | 45.411 | 26.595 | 1.00 | 0.00 |
| ATOM | 2082 | C | ASP | 1 | 59 | 29.115 | 45.537 | 26.531 | 1.00 | 0.00 |
| ATOM | 2083 | O | ASP | 1 | 59 | 29.777 | 44.557 | 26.222 | 1.00 | 0.00 |
| ATOM | 2084 | CB | ASP | 1 | 59 | 26.967 | 45.581 | 28.001 | 1.00 | 0.00 |
| ATOM | 2085 | CG | ASP | 1 | 59 | 27.505 | 46.766 | 28.779 | 1.00 | 0.00 |
| ATOM | 2086 | OD1 | ASP | 1 | 59 | 26.994 | 47.872 | 28.690 | 1.00 | 0.00 |
| ATOM | 2087 | OD2 | ASP | 1 | 59 | 28.492 | 46.600 | 29.480 | 1.00 | 0.00 |
| ATOM | 2088 | H | ASP | 1 | 59 | 26.735 | 43.438 | 26.752 | 1.00 | 0.00 |
| ATOM | 2089 | N | GLY | 1 | 60 | 29.692 | 46.718 | 26.838 | 1.00 | 0.00 |
| ATOM | 2090 | CA | GLY | 1 | 60 | 31.143 | 46.911 | 26.704 | 1.00 | 0.00 |
| ATOM | 2091 | C | GLY | 1 | 60 | 31.910 | 46.976 | 28.022 | 1.00 | 0.00 |
| ATOM | 2092 | O | GLY | 1 | 60 | 33.034 | 47.460 | 28.135 | 1.00 | 0.00 |
| ATOM | 2093 | H | GLY | 1 | 60 | 29.076 | 47.437 | 27.153 | 1.00 | 0.00 |
| ATOM | 2094 | N | LYS | 1 | 61 | 31.238 | 46.456 | 29.052 | 1.00 | 0.00 |
| ATOM | 2095 | CA | LYS | 1 | 61 | 31.826 | 46.305 | 30.392 | 1.00 | 0.00 |
| ATOM | 2096 | C | LYS | 1 | 61 | 31.514 | 44.929 | 30.954 | 1.00 | 0.00 |
| ATOM | 2097 | O | LYS | 1 | 61 | 32.333 | 44.249 | 31.562 | 1.00 | 0.00 |
| ATOM | 2098 | CB | LYS | 1 | 61 | 31.344 | 47.405 | 31.343 | 1.00 | 0.00 |
| ATOM | 2099 | CG | LYS | 1 | 61 | 31.823 | 48.793 | 30.905 | 1.00 | 0.00 |
| ATOM | 2100 | CD | LYS | 1 | 61 | 30.849 | 49.923 | 31.249 | 1.00 | 0.00 |
| ATOM | 2101 | CE | LYS | 1 | 61 | 29.407 | 49.631 | 30.813 | 1.00 | 0.00 |
| ATOM | 2102 | NZ | LYS | 1 | 61 | 29.337 | 49.205 | 29.416 | 1.00 | 0.00 |
| ATOM | 2103 | H | LYS | 1 | 61 | 30.272 | 46.270 | 28.900 | 1.00 | 0.00 |
| ATOM | 2104 | 1HZ | LYS | 1 | 61 | 30.233 | 48.774 | 29.139 | 1.00 | 0.00 |
| ATOM | 2105 | 2HZ | LYS | 1 | 61 | 28.590 | 48.483 | 29.335 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2106 | 3HZ | LYS | 1 | 61 | 29.119 | 49.993 | 28.783 | 1.00 | 0.00 |
| ATOM | 2107 | N | TYR | 1 | 62 | 30.286 | 44.482 | 30.615 | 1.00 | 0.00 |
| ATOM | 2108 | CA | TYR | 1 | 62 | 30.141 | 43.031 | 30.501 | 1.00 | 0.00 |
| ATOM | 2109 | C | TYR | 1 | 62 | 31.020 | 42.477 | 29.378 | 1.00 | 0.00 |
| ATOM | 2110 | O | TYR | 1 | 62 | 31.826 | 41.570 | 29.556 | 1.00 | 0.00 |
| ATOM | 2111 | CB | TYR | 1 | 62 | 28.643 | 42.644 | 30.381 | 1.00 | 0.00 |
| ATOM | 2112 | CG | TYR | 1 | 62 | 28.438 | 41.432 | 39.492 | 1.00 | 0.00 |
| ATOM | 2113 | CD1 | TYR | 1 | 62 | 27,965 | 41.655 | 28.186 | 1.00 | 0.00 |
| ATOM | 2114 | CD2 | TYR | 1 | 62 | 28.788 | 40.141 | 29.946 | 1.00 | 0.00 |
| ATOM | 2115 | CE1 | TYR | 1 | 62 | 27.990 | 40.600 | 27.265 | 1.00 | 0.00 |
| ATOM | 2116 | CE2 | TYR | 1 | 62 | 28.806 | 39.081 | 29.022 | 1.00 | 0.00 |
| ATOM | 2117 | CZ | TYR | 1 | 62 | 28.463 | 39.343 | 27.679 | 1.00 | 0.00 |
| ATOM | 2118 | OH | TYR | 1 | 62 | 28.625 | 38.359 | 26.722 | 1.00 | 0.00 |
| ATOM | 2119 | H | TYR | 1 | 62 | 29.552 | 45.085 | 30.301 | 1.00 | 0.00 |
| ATOM | 2120 | HH | TYR | 1 | 62 | 28.154 | 37.570 | 27.009 | 1.00 | 0.00 |
| ATOM | 2121 | N | GLY | 1 | 63 | 30.851 | 43.057 | 28.188 | 1.00 | 0.00 |
| ATOM | 2122 | CA | GLY | 1 | 63 | 31.674 | 42.548 | 27.089 | 1.00 | 0.00 |
| ATOM | 2123 | C | GLY | 1 | 63 | 32.965 | 43.312 | 26.911 | 1.00 | 0.00 |
| ATOM | 2124 | O | GLY | 1 | 63 | 33.559 | 43.350 | 25.836 | 1.00 | 0.00 |
| ATOM | 2125 | H | GLY | 1 | 63 | 20.177 | 43.782 | 28.051 | 1.00 | 0.00 |
| ATOM | 2126 | N | ALA | 1 | 64 | 33.409 | 43.868 | 28.062 | 1.00 | 0.00 |
| ATOM | 2127 | CA | ALA | 1 | 64 | 34.805 | 44.289 | 28.103 | 1.00 | 0.00 |
| ATOM | 2128 | C | ALA | 1 | 64 | 35.716 | 43.095 | 27.917 | 1.00 | 0.00 |
| ATOM | 2129 | O | ALA | 1 | 64 | 36.748 | 43.174 | 27.272 | 1.00 | 0.00 |
| ATOM | 2130 | CB | ALA | 1 | 64 | 35.142 | 44.959 | 29.434 | 1.00 | 0.00 |
| ATOM | 2131 | H | ALA | 1 | 64 | 32.920 | 43.717 | 28.916 | 1.00 | 0.00 |
| ATOM | 2132 | N | ARG | 1 | 65 | 35.218 | 41.933 | 28.420 | 1.00 | 0.00 |
| ATOM | 2133 | CA | ARG | 1 | 65 | 35.967 | 40.675 | 28.267 | 1.00 | 0.00 |
| ATOM | 2134 | C | ARG | 1 | 65 | 36.173 | 40.123 | 26.845 | 1.00 | 0.00 |
| ATOM | 2135 | O | ARG | 1 | 65 | 36.498 | 38.956 | 26.625 | 1.00 | 0.00 |
| ATOM | 2136 | CB | ARG | 1 | 65 | 35.450 | 39.618 | 29.278 | 1.00 | 0.00 |
| ATOM | 2137 | CG | ARG | 1 | 65 | 34.476 | 38.519 | 28.807 | 1.00 | 0.00 |
| ATOM | 2138 | CD | ARG | 1 | 65 | 33.220 | 39.070 | 28.134 | 1.00 | 0.00 |
| ATOM | 2139 | NE | ARG | 1 | 65 | 32.486 | 38.097 | 27.327 | 1.00 | 0.00 |
| ATOM | 2140 | CZ | ARG | 1 | 65 | 32.827 | 37.913 | 26.025 | 1.00 | 0.00 |
| ATOM | 2141 | NH1 | ARG | 1 | 65 | 31.908 | 37.560 | 25.143 | 1.00 | 0.00 |
| ATOM | 2142 | NH2 | ARG | 1 | 65 | 34.057 | 38.120 | 25.572 | 1.00 | 0.00 |
| ATOM | 2143 | H | ARG | 1 | 65 | 34.359 | 42.009 | 28.928 | 1.00 | 0.00 |
| ATOM | 2144 | HE | ARG | 1 | 65 | 31.613 | 37.735 | 27.656 | 1.00 | 0.00 |
| ATOM | 2145 | 1HH1 | ARG | 1 | 65 | 32.170 | 37.531 | 24.178 | 1.00 | 0.00 |
| ATOM | 2146 | 2HH1 | ARG | 1 | 65 | 30.970 | 37.352 | 25.419 | 1.00 | 0.00 |
| ATOM | 2147 | 1HH2 | ARG | 1 | 65 | 34.207 | 38.219 | 24.578 | 1.00 | 0.00 |
| ATOM | 2148 | 2HH2 | ARG | 1 | 65 | 34.850 | 38.202 | 26.178 | 1.00 | 0.00 |
| ATOM | 2149 | N | ASP | 1 | 66 | 35.896 | 40.978 | 25.853 | 1.00 | 0.00 |
| ATOM | 2150 | CA | ASP | 1 | 66 | 36.121 | 40.556 | 24.472 | 1.00 | 0.00 |
| ATOM | 2151 | C | ASP | 1 | 66 | 37.546 | 40.632 | 23.899 | 1.00 | 0.00 |
| ATOM | 2152 | O | ASP | 1 | 66 | 38.069 | 39.600 | 23.474 | 1.00 | 0.00 |
| ATOM | 2153 | CB | ASP | 1 | 66 | 35.018 | 41.132 | 23.566 | 1.00 | 0.00 |
| ATOM | 2154 | CG | ASP | 1 | 66 | 34.022 | 40.038 | 23.253 | 1.00 | 0.00 |
| ATOM | 2155 | OD1 | ASP | 1 | 66 | 32.994 | 40.080 | 23.719 | 1.00 | 0.00 |
| ATOM | 2156 | OD2 | ASP | 1 | 66 | 34.397 | 39.109 | 22.558 | 1.00 | 0.00 |
| ATOM | 2157 | H | ASP | 1 | 66 | 35.708 | 41.943 | 26.032 | 1.00 | 0.00 |
| ATOM | 2158 | N | PRO | 1 | 67 | 38.197 | 41.829 | 23.900 | 1.00 | 0.00 |
| ATOM | 2159 | CA | PRO | 1 | 67 | 39.592 | 41.943 | 23.431 | 1.00 | 0.00 |
| ATOM | 2160 | C | PRO | 1 | 67 | 40.542 | 40.772 | 23.697 | 1.00 | 0.00 |
| ATOM | 2161 | O | PRO | 1 | 67 | 41.195 | 40.190 | 22.821 | 1.00 | 0.00 |
| ATOM | 2162 | CB | PRO | 1 | 67 | 40.039 | 43.191 | 24.185 | 1.00 | 0.00 |
| ATOM | 2163 | CG | PRO | 1 | 67 | 38.815 | 44.096 | 24.270 | 1.00 | 0.00 |
| ATOM | 2164 | CD | PRO | 1 | 67 | 37.663 | 43.116 | 24.342 | 1.00 | 0.00 |
| ATOM | 2165 | N | GLU | 1 | 68 | 40.582 | 40.505 | 25.014 | 1.00 | 0.00 |
| ATOM | 2166 | CA | GLU | 1 | 68 | 41.552 | 39.535 | 25.674 | 1.00 | 0.00 |
| ATOM | 2167 | C | GLU | 1 | 68 | 41.507 | 38.206 | 25.177 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2168 | O | GLU | 1 | 68 | 42.484 | 37.464 | 25.113 | 1.00 | 0.00 |
| ATOM | 2169 | CB | GLU | 1 | 68 | 41.334 | 39.636 | 27.200 | 1.00 | 0.00 |
| ATOM | 2170 | CG | GLU | 1 | 68 | 40.996 | 40.976 | 27.886 | 1.00 | 0.00 |
| ATOM | 2171 | CD | GLU | 1 | 68 | 39.489 | 41.159 | 28.050 | 1.00 | 0.00 |
| ATOM | 2172 | OE1 | GLU | 1 | 68 | 38.980 | 41.005 | 29.158 | 1.00 | 0.00 |
| ATOM | 2173 | OE2 | GLU | 1 | 68 | 38.802 | 41.457 | 27.078 | 1.00 | 0.00 |
| ATOM | 2174 | H | GLU | 1 | 68 | 39.884 | 40.900 | 25.604 | 1.00 | 0.00 |
| ATOM | 2175 | N | THR | 1 | 69 | 40.284 | 37.824 | 24.803 | 1.00 | 0.00 |
| ATOM | 2176 | CA | THR | 1 | 69 | 40.084 | 36.472 | 24.295 | 1.00 | 0.00 |
| ATOM | 2177 | C | THR | 1 | 69 | 40.920 | 36.110 | 23.056 | 1.00 | 0.00 |
| ATOM | 2178 | O | THR | 1 | 69 | 41.215 | 34.952 | 22.749 | 1.00 | 0.00 |
| ATOM | 2179 | CB | THR | 1 | 69 | 38.564 | 36.229 | 24.163 | 1.00 | 0.00 |
| ATOM | 2180 | OG1 | THR | 1 | 69 | 38.197 | 34.952 | 24.692 | 1.00 | 0.00 |
| ATOM | 2181 | CG2 | THR | 1 | 69 | 37.988 | 36.443 | 22.761 | 1.00 | 0.00 |
| ATOM | 2182 | H | THR | 1 | 69 | 39.531 | 38.466 | 24.924 | 1.00 | 0.00 |
| ATOM | 2183 | HG1 | THR | 1 | 69 | 37.248 | 34.948 | 24.706 | 1.00 | 0.00 |
| ATOM | 2184 | N | LYS | 1 | 70 | 41.354 | 37.171 | 22.347 | 1.00 | 0.00 |
| ATOM | 2185 | CA | LYS | 1 | 70 | 42.185 | 36.868 | 21.187 | 1.00 | 0.00 |
| ATOM | 2186 | C | LYS | 1 | 70 | 43.665 | 36.656 | 21.455 | 1.00 | 0.00 |
| ATOM | 2187 | O | LYS | 1 | 70 | 44.531 | 37.349 | 20.916 | 1.00 | 0.00 |
| ATOM | 2188 | CB | LYS | 1 | 70 | 41.956 | 37.879 | 20.061 | 1.00 | 0.00 |
| ATOM | 2189 | CG | LYS | 1 | 70 | 42.149 | 37.240 | 18.681 | 1.00 | 0.00 |
| ATOM | 2190 | CD | LYS | 1 | 70 | 41.757 | 38.167 | 17.539 | 1.00 | 0.00 |
| ATOM | 2191 | CE | LYS | 1 | 70 | 41.412 | 37.473 | 16.222 | 1.00 | 0.00 |
| ATOM | 2192 | NZ | LYS | 1 | 70 | 40.366 | 38.264 | 15.549 | 1.00 | 0.00 |
| ATOM | 2193 | H | LYS | 1 | 70 | 41.220 | 38.100 | 22.702 | 1.00 | 0.00 |
| ATOM | 2194 | 1HZ | LYS | 1 | 70 | 39.454 | 38.204 | 16.058 | 1.00 | 0.00 |
| ATOM | 2195 | 2HZ | LYS | 1 | 70 | 40.641 | 39.264 | 15.469 | 1.00 | 0.00 |
| ATOM | 2196 | 3HZ | LYS | 1 | 70 | 40.234 | 37.973 | 14.557 | 1.00 | 0.00 |
| ATOM | 2197 | N | ILE | 1 | 71 | 43.929 | 35.626 | 22.269 | 1.00 | 0.00 |
| ATOM | 2198 | CA | ILE | 1 | 71 | 45.257 | 35.047 | 22.119 | 1.00 | 0.00 |
| ATOM | 2199 | C | ILE | 1 | 71 | 45.258 | 34.062 | 20.953 | 1.00 | 0.00 |
| ATOM | 2200 | O | ILE | 1 | 71 | 46.208 | 33.939 | 20.181 | 1.00 | 0.00 |
| ATOM | 2201 | CB | ILE | 1 | 71 | 45.762 | 34.455 | 23.451 | 1.00 | 0.00 |
| ATOM | 2202 | CG1 | ILE | 1 | 71 | 47.203 | 33.946 | 23.338 | 1.00 | 0.00 |
| ATOM | 2203 | CG2 | ILE | 1 | 71 | 44.831 | 33.361 | 23.991 | 1.00 | 0.00 |
| ATOM | 2204 | CD1 | ILE | 1 | 71 | 47.789 | 33.493 | 24.677 | 1.00 | 0.00 |
| ATOM | 2205 | H | ILE | 1 | 71 | 43.182 | 35.175 | 22.755 | 1.00 | 0.00 |
| ATOM | 2206 | N | TRP | 1 | 72 | 44.108 | 33.384 | 20.829 | 1.00 | 0.00 |
| ATOM | 2207 | CA | TRP | 1 | 72 | 43.848 | 32.812 | 19.516 | 1.00 | 0.00 |
| ATOM | 2208 | C | TRP | 1 | 72 | 42.642 | 33.491 | 18.896 | 1.00 | 0.00 |
| ATOM | 2209 | O | TRP | 1 | 72 | 42.777 | 34.298 | 17.976 | 1.00 | 0.00 |
| ATOM | 2210 | CB | TRP | 1 | 72 | 43.833 | 31.267 | 19.530 | 1.00 | 0.00 |
| ATOM | 2211 | CG | TRP | 1 | 72 | 42.984 | 30.636 | 20.619 | 1.00 | 0.00 |
| ATOM | 2212 | CD1 | TRP | 1 | 72 | 43.310 | 30.473 | 21.973 | 1.00 | 0.00 |
| ATOM | 2213 | CD2 | TRP | 1 | 72 | 41.685 | 30.027 | 20.471 | 1.00 | 0.00 |
| ATOM | 2214 | NE1 | TRP | 1 | 72 | 42.322 | 29.222 | 22.653 | 1.00 | 0.00 |
| ATOM | 2215 | CE2 | TRP | 1 | 72 | 41.300 | 29.527 | 21.759 | 1.00 | 0.00 |
| ATOM | 2216 | CE3 | TRP | 1 | 72 | 40.826 | 39.859 | 19.364 | 1.00 | 0.00 |
| ATOM | 2217 | CZ2 | TRP | 1 | 72 | 40.064 | 28.866 | 21.914 | 1.00 | 0.00 |
| ATOM | 2218 | CZ3 | TRP | 1 | 72 | 39.593 | 29.196 | 19.533 | 1.00 | 0.00 |
| ATOM | 2219 | CH2 | TRP | 1 | 72 | 39.216 | 28.701 | 20.800 | 1.00 | 0.00 |
| ATOM | 2220 | H | TRP | 1 | 72 | 43.394 | 33.444 | 21.537 | 1.00 | 0.00 |
| ATOM | 2221 | HE1 | TRP | 1 | 72 | 42.321 | 29.552 | 23.607 | 1.00 | 0.00 |
| ATOM | 2222 | N | ASN | 1 | 73 | 41.499 | 33.209 | 19.528 | 1.00 | 0.00 |
| ATOM | 2223 | CA | ASN | 1 | 73 | 40.222 | 33.910 | 19.366 | 1.00 | 0.00 |
| ATOM | 2224 | C | ASN | 1 | 73 | 39.186 | 33.137 | 20.130 | 1.00 | 0.00 |
| ATOM | 2225 | O | ASN | 1 | 73 | 38.426 | 32.343 | 19.588 | 1.00 | 0.00 |
| ATOM | 2226 | CB | ASN | 1 | 73 | 39.741 | 34.167 | 17.923 | 1.00 | 0.00 |
| ATOM | 2227 | CG | ASN | 1 | 73 | 40.039 | 33.060 | 16.927 | 1.00 | 0.00 |
| ATOM | 2228 | OD1 | ASN | 1 | 73 | 40.930 | 33.198 | 16.092 | 1.00 | 0.00 |
| ATOM | 2229 | ND2 | ASN | 1 | 73 | 39.245 | 31.992 | 16.985 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2230 | H | ASN | 1 | 73 | 41.534 | 32.510 | 20.237 | 1.00 | 0.00 |
| ATOM | 2231 | 1HD2 | ASN | 1 | 73 | 39.388 | 31.186 | 16.408 | 1.00 | 0.00 |
| ATOM | 2232 | 2HD2 | ASN | 1 | 73 | 38.497 | 31.978 | 17.653 | 1.00 | 0.00 |
| ATOM | 2233 | N | GLY | 1 | 74 | 39.273 | 33.332 | 21.444 | 1.00 | 0.00 |
| ATOM | 2234 | CA | GLY | 1 | 74 | 38.442 | 32.542 | 22.335 | 1.00 | 0.00 |
| ATOM | 2235 | C | GLY | 1 | 74 | 39.062 | 32.366 | 23.705 | 1.00 | 0.00 |
| ATOM | 2236 | O | GLY | 1 | 74 | 39.390 | 32.343 | 24.727 | 1.00 | 0.00 |
| ATOM | 2237 | H | GLY | 1 | 74 | 38.825 | 34.087 | 21.794 | 1.00 | 0.00 |
| ATOM | 2238 | N | MET | 1 | 75 | 40.403 | 32.242 | 23.684 | 1.00 | 0.00 |
| ATOM | 2239 | CA | MET | 1 | 75 | 41.184 | 32.010 | 24.902 | 1.00 | 0.00 |
| ATOM | 2240 | C | MET | 1 | 75 | 40.800 | 30.739 | 25.649 | 1.00 | 0.00 |
| ATOM | 2241 | O | MET | 1 | 75 | 41.346 | 29.679 | 25.372 | 1.00 | 0.00 |
| ATOM | 2242 | CB | MET | 1 | 75 | 41.227 | 33.277 | 25.775 | 1.00 | 0.00 |
| ATOM | 2243 | CG | MET | 1 | 75 | 42.241 | 33.264 | 26.923 | 1.00 | 0.00 |
| ATOM | 2244 | SD | MET | 1 | 75 | 42.287 | 34.841 | 27.793 | 1.00 | 0.00 |
| ATOM | 2245 | CE | MET | 1 | 75 | 40.546 | 34.918 | 28.260 | 1.00 | 0.00 |
| ATOM | 2246 | H | MET | 1 | 75 | 40.859 | 32.359 | 22.805 | 1.00 | 0.00 |
| ATOM | 2247 | N | VAL | 1 | 76 | 39.855 | 30.896 | 26.580 | 1.00 | 0.00 |
| ATOM | 2248 | CA | VAL | 1 | 76 | 39.390 | 29.729 | 27.311 | 1.00 | 0.00 |
| ATOM | 2249 | C | VAL | 1 | 76 | 38.045 | 29.219 | 26.825 | 1.00 | 0.00 |
| ATOM | 2250 | O | VAL | 1 | 76 | 37.466 | 28.322 | 27.428 | 1.00 | 0.00 |
| ATOM | 2251 | CB | VAL | 1 | 76 | 39.357 | 30.020 | 28.818 | 1.00 | 0.00 |
| ATOM | 2252 | CG1 | VAL | 1 | 76 | 40.774 | 30.221 | 29.360 | 1.00 | 0.00 |
| ATOM | 2253 | CG2 | VAL | 1 | 76 | 38.439 | 31.200 | 29.161 | 1.00 | 0.00 |
| ATOM | 2254 | H | VAL | 1 | 76 | 39.329 | 31.746 | 26.631 | 1.00 | 0.00 |
| ATOM | 2255 | N | GLY | 1 | 77 | 37.580 | 29.824 | 25.734 | 1.00 | 0.00 |
| ATOM | 2256 | CA | GLY | 1 | 77 | 36.281 | 29.491 | 25.175 | 1.00 | 0.00 |
| ATOM | 2257 | C | GLY | 1 | 77 | 36.395 | 29.339 | 23.675 | 1.00 | 0.00 |
| ATOM | 2258 | O | GLY | 1 | 77 | 37.394 | 29.800 | 23.027 | 1.00 | 0.00 |
| ATOM | 2259 | H | GLY | 1 | 77 | 38.093 | 30.550 | 25.288 | 1.00 | 0.00 |
| ATOM | 2260 | N | GLU | 1 | 78 | 35.406 | 28.624 | 23.141 | 1.00 | 0.00 |
| ATOM | 2261 | CA | GLU | 1 | 78 | 35.566 | 28.205 | 21.756 | 1.00 | 0.00 |
| ATOM | 2262 | C | GLU | 1 | 78 | 35.307 | 29.293 | 20.747 | 1.00 | 0.00 |
| ATOM | 2263 | O | GLU | 1 | 78 | 34.448 | 30.159 | 20.896 | 1.00 | 0.00 |
| ATOM | 2264 | CB | GLU | 1 | 78 | 34.716 | 26.982 | 21.378 | 1.00 | 0.00 |
| ATOM | 2265 | CG | GLU | 1 | 78 | 34.756 | 25.791 | 22.342 | 1.00 | 0.00 |
| ATOM | 2266 | CD | GLU | 1 | 78 | 33.970 | 26.144 | 23.585 | 1.00 | 0.00 |
| ATOM | 2267 | OE1 | GLU | 1 | 78 | 34.561 | 26.219 | 24.657 | 1.00 | 0.00 |
| ATOM | 2268 | OE2 | GLU | 1 | 78 | 32.777 | 26.396 | 23.472 | 1.00 | 0.00 |
| ATOM | 2269 | H | GLU | 1 | 78 | 34.668 | 28.228 | 23.698 | 1.00 | 0.00 |
| ATOM | 2270 | N | LEU | 1 | 79 | 36.118 | 29.150 | 19.686 | 1.00 | 0.00 |
| ATOM | 2271 | CA | LEU | 1 | 79 | 35.981 | 29.844 | 18.401 | 1.00 | 0.00 |
| ATOM | 2272 | C | LEU | 1 | 79 | 35.178 | 31.129 | 18.369 | 1.00 | 0.00 |
| ATOM | 2273 | O | LEU | 1 | 79 | 34.211 | 31.299 | 17.632 | 1.00 | 0.00 |
| ATOM | 2274 | CB | LEU | 1 | 79 | 35.475 | 28.869 | 17.334 | 1.00 | 0.00 |
| ATOM | 2275 | CG | LEU | 1 | 79 | 36.444 | 27.717 | 17.057 | 1.00 | 0.00 |
| ATOM | 2276 | CD1 | LEU | 1 | 79 | 35.802 | 20.639 | 16.184 | 1.00 | 0.00 |
| ATOM | 2277 | CD2 | LEU | 1 | 79 | 37.769 | 28.211 | 16.470 | 1.00 | 0.00 |
| ATOM | 2278 | H | LEU | 1 | 79 | 36.350 | 28.484 | 19.804 | 1.00 | 0.00 |
| ATOM | 2279 | N | VAL | 1 | 80 | 35.630 | 32.072 | 19.204 | 1.00 | 0.00 |
| ATOM | 2280 | CA | VAL | 1 | 80 | 35.032 | 33.404 | 19.121 | 1.00 | 0.00 |
| ATOM | 2281 | C | VAL | 1 | 80 | 35.583 | 34.087 | 17.922 | 1.00 | 0.00 |
| ATOM | 2282 | O | VAL | 1 | 80 | 36.643 | 33.504 | 17.357 | 1.00 | 0.00 |
| ATOM | 2283 | CB | VAL | 1 | 80 | 35.259 | 34.151 | 20.460 | 1.00 | 0.00 |
| ATOM | 2284 | CG1 | VAL | 1 | 80 | 34.492 | 35.471 | 20.594 | 1.00 | 0.00 |
| ATOM | 2285 | CG2 | VAL | 1 | 80 | 34.882 | 33.259 | 21.644 | 1.00 | 0.00 |
| ATOM | 2286 | H | VAL | 1 | 80 | 36.450 | 31.889 | 19.750 | 1.00 | 0.00 |
| ATOM | 2287 | N | TYR | 1 | 81 | 35.180 | 35.266 | 17.529 | 1.00 | 0.00 |
| ATOM | 2288 | CA | TYR | 1 | 81 | 36.018 | 35.987 | 16.563 | 1.00 | 0.00 |
| ATOM | 2289 | C | TYR | 1 | 81 | 37.255 | 36.637 | 17.186 | 1.00 | 0.00 |
| ATOM | 2290 | O | TYR | 1 | 81 | 38.301 | 36.815 | 15.563 | 1.00 | 0.00 |
| ATOM | 2291 | CB | TYR | 1 | 81 | 35.197 | 37.016 | 15.768 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2292 | CG | TYR | 1 | 81 | 35.546 | 37.002 | 14.289 | 1.00 | 0.00 |
| ATOM | 2293 | CD1 | TYR | 1 | 81 | 36.572 | 37.837 | 13.792 | 1.00 | 0.00 |
| ATOM | 2294 | CD2 | TYR | 1 | 81 | 34.813 | 36.155 | 13.432 | 1.00 | 0.00 |
| ATOM | 2295 | CE1 | TYR | 1 | 81 | 36.856 | 37.834 | 12.412 | 1.00 | 0.00 |
| ATOM | 2296 | CE2 | TYR | 1 | 81 | 35.096 | 36.153 | 12.054 | 1.00 | 0.00 |
| ATOM | 2297 | CZ | TYR | 1 | 81 | 36.113 | 36.993 | 11.553 | 1.00 | 0.00 |
| ATOM | 2298 | OH | TYR | 1 | 81 | 36.389 | 36.981 | 10.191 | 1.00 | 0.00 |
| ATOM | 2299 | H | TYR | 1 | 81 | 34.409 | 35.628 | 18.053 | 1.00 | 0.00 |
| ATOM | 2300 | HH | TYR | 1 | 81 | 35.739 | 36.425 | 9.769 | 1.00 | 0.00 |
| ATOM | 2301 | N | GLY | 1 | 82 | 37.077 | 37.034 | 18.467 | 1.00 | 0.00 |
| ATOM | 2302 | CA | GLY | 1 | 82 | 38.061 | 37.767 | 19.272 | 1.00 | 0.00 |
| ATOM | 2303 | C | GLY | 1 | 82 | 38.578 | 39.052 | 18.644 | 1.00 | 0.00 |
| ATOM | 2304 | O | GLY | 1 | 82 | 38.626 | 39.162 | 17.425 | 1.00 | 0.00 |
| ATOM | 2305 | H | GLY | 1 | 82 | 36.267 | 36.675 | 18.928 | 1.00 | 0.00 |
| ATOM | 2306 | N | ARG | 1 | 83 | 39.015 | 39.989 | 19.504 | 1.00 | 0.00 |
| ATOM | 2307 | CA | ARG | 1 | 83 | 39.344 | 41.334 | 18.995 | 1.00 | 0.00 |
| ATOM | 2308 | C | ARG | 1 | 83 | 38.075 | 42.004 | 18.513 | 1.00 | 0.00 |
| ATOM | 2309 | O | ARG | 1 | 83 | 37.854 | 42.288 | 17.333 | 1.00 | 0.00 |
| ATOM | 2310 | CB | ARG | 1 | 83 | 40.424 | 41.330 | 17.888 | 1.00 | 0.00 |
| ATOM | 2311 | CG | ARG | 1 | 83 | 41.021 | 42.634 | 17.362 | 1.00 | 0.00 |
| ATOM | 2312 | CD | ARG | 1 | 83 | 42.250 | 43.053 | 18.153 | 1.00 | 0.00 |
| ATOM | 2313 | NE | ARG | 1 | 83 | 41.876 | 43.367 | 19.522 | 1.00 | 0.00 |
| ATOM | 2314 | CZ | ARG | 1 | 83 | 42.748 | 43.324 | 20.524 | 1.00 | 0.00 |
| ATOM | 2315 | NH1 | ARG | 1 | 83 | 42.380 | 43.815 | 21.689 | 1.00 | 0.00 |
| ATOM | 2316 | NH2 | ARG | 1 | 83 | 43.954 | 42.813 | 20.356 | 1.00 | 0.00 |
| ATOM | 2317 | H | ARG | 1 | 83 | 38.898 | 39.842 | 20.492 | 1.00 | 0.00 |
| ATOM | 2318 | HE | ARG | 1 | 83 | 40.980 | 43.792 | 19.690 | 1.00 | 0.00 |
| ATOM | 2319 | 1HH1 | ARG | 1 | 83 | 42.993 | 43.898 | 22.480 | 1.00 | 0.00 |
| ATOM | 2320 | 2HH1 | ARG | 1 | 83 | 41.438 | 44.163 | 21.786 | 1.00 | 0.00 |
| ATOM | 2321 | 1HH2 | ARG | 1 | 83 | 44.612 | 42.903 | 21.107 | 1.00 | 0.00 |
| ATOM | 2322 | 2HH2 | ARG | 1 | 83 | 44.209 | 42.358 | 19.502 | 1.00 | 0.00 |
| ATOM | 2323 | N | ALA | 1 | 84 | 37.229 | 42.210 | 19.526 | 1.00 | 0.00 |
| ATOM | 2324 | CA | ALA | 1 | 84 | 35.009 | 42.931 | 19.198 | 1.00 | 0.00 |
| ATOM | 2325 | C | ALA | 1 | 84 | 36.211 | 44.436 | 19.209 | 1.00 | 0.00 |
| ATOM | 2326 | O | ALA | 1 | 84 | 35.283 | 45.239 | 19.140 | 1.00 | 0.00 |
| ATOM | 2327 | CB | ALA | 1 | 84 | 34.895 | 42.546 | 20.166 | 1.00 | 0.00 |
| ATOM | 2328 | H | ALA | 1 | 84 | 37.555 | 42.163 | 20.470 | 1.00 | 0.00 |
| ATOM | 2329 | N | ASP | 1 | 85 | 37.474 | 44.801 | 19.350 | 1.00 | 0.00 |
| ATOM | 2330 | CA | ASP | 1 | 85 | 37.826 | 46.195 | 19.452 | 1.00 | 0.00 |
| ATOM | 2331 | C | ASP | 1 | 85 | 38.557 | 46.627 | 18.191 | 1.00 | 0.00 |
| ATOM | 2332 | O | ASP | 1 | 85 | 38.290 | 46.079 | 17.122 | 1.00 | 0.00 |
| ATOM | 2333 | CB | ASP | 1 | 85 | 38.573 | 46.417 | 20.762 | 1.00 | 0.00 |
| ATOM | 2334 | CG | ASP | 1 | 85 | 39.734 | 45.475 | 20.737 | 1.00 | 0.00 |
| ATOM | 2335 | OD1 | ASP | 1 | 85 | 39.606 | 44.374 | 21.238 | 1.00 | 0.00 |
| ATOM | 2336 | OD2 | ASP | 1 | 85 | 40.747 | 45.814 | 20.159 | 1.00 | 0.00 |
| ATOM | 2337 | H | ASP | 1 | 85 | 38.224 | 44.146 | 19.311 | 1.00 | 0.00 |
| ATOM | 2338 | N | ILE | 1 | 86 | 39.384 | 47.685 | 18.347 | 1.00 | 0.00 |
| ATOM | 2339 | CA | ILE | 1 | 86 | 39.157 | 48.916 | 17.575 | 1.00 | 0.00 |
| ATOM | 2340 | C | ILE | 1 | 86 | 37.773 | 49.537 | 17.774 | 1.00 | 0.00 |
| ATOM | 2341 | O | ILE | 1 | 86 | 37.162 | 50.185 | 16.906 | 1.00 | 0.00 |
| ATOM | 2342 | CB | ILE | 1 | 86 | 39.668 | 48.843 | 16.115 | 1.00 | 0.00 |
| ATOM | 2343 | CG1 | ILE | 1 | 86 | 40.258 | 50.192 | 15.699 | 1.00 | 0.00 |
| ATOM | 2344 | CG2 | ILE | 1 | 86 | 38.618 | 48.386 | 15.093 | 1.00 | 0.00 |
| ATOM | 2345 | CD1 | ILE | 1 | 86 | 41.075 | 50.113 | 14.408 | 1.00 | 0.00 |
| ATOM | 2346 | H | ILE | 1 | 86 | 39.852 | 47.802 | 19.223 | 1.00 | 0.00 |
| ATOM | 2347 | N | ALA | 1 | 87 | 37.333 | 49.268 | 19.016 | 1.00 | 0.00 |
| ATOM | 2348 | CA | ALA | 1 | 87 | 36.039 | 49.687 | 19.501 | 1.00 | 0.00 |
| ATOM | 2349 | C | ALA | 1 | 87 | 36.043 | 51.170 | 19.531 | 1.00 | 0.00 |
| ATOM | 2350 | O | ALA | 1 | 87 | 36.694 | 51.799 | 20.360 | 1.00 | 0.00 |
| ATOM | 2351 | CB | ALA | 1 | 87 | 35.800 | 49.169 | 20.924 | 1.00 | 0.00 |
| ATOM | 2352 | H | ALA | 1 | 87 | 38.072 | 48.996 | 19.622 | 1.00 | 0.00 |
| ATOM | 2353 | N | VAL | 1 | 88 | 35.332 | 51.716 | 18.549 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2354 | CA | VAL | 1 | 88 | 34.934 | 53.110 | 18.743 | 1.00 | 0.00 |
| ATOM | 2355 | C | VAL | 1 | 88 | 33.694 | 53.094 | 19.551 | 1.00 | 0.00 |
| ATOM | 2356 | O | VAL | 1 | 88 | 33.071 | 52.037 | 19.653 | 1.00 | 0.00 |
| ATOM | 2357 | CB | VAL | 1 | 88 | 34.906 | 53.837 | 17.391 | 1.00 | 0.00 |
| ATOM | 2358 | CG1 | VAL | 1 | 88 | 35.001 | 55.354 | 17.548 | 1.00 | 0.00 |
| ATOM | 2359 | CG2 | VAL | 1 | 88 | 36.041 | 53.381 | 16.468 | 1.00 | 0.00 |
| ATOM | 2360 | H | VAL | 1 | 88 | 34.894 | 51.169 | 17.838 | 1.00 | 0.00 |
| ATOM | 2361 | N | ALA | 1 | 89 | 33.396 | 54.262 | 20.152 | 1.00 | 0.00 |
| ATOM | 2362 | CA | ALA | 1 | 89 | 32.414 | 54.462 | 21.229 | 1.00 | 0.00 |
| ATOM | 2363 | C | ALA | 1 | 89 | 33.088 | 54.623 | 22.566 | 1.00 | 0.00 |
| ATOM | 2364 | O | ALA | 1 | 89 | 33.818 | 53.770 | 23.065 | 1.00 | 0.00 |
| ATOM | 2365 | CB | ALA | 1 | 89 | 31.333 | 53.388 | 21.417 | 1.00 | 0.00 |
| ATOM | 2366 | H | ALA | 1 | 89 | 34.071 | 54.986 | 20.015 | 1.00 | 0.00 |
| ATOM | 2367 | N | PRO | 1 | 90 | 32.789 | 54.799 | 23.165 | 1.00 | 0.00 |
| ATOM | 2368 | CA | PRO | 1 | 90 | 33.416 | 56.268 | 24.407 | 1.00 | 0.00 |
| ATOM | 2369 | C | PRO | 1 | 90 | 33.771 | 55.286 | 25.517 | 1.00 | 0.00 |
| ATOM | 2370 | O | PRO | 1 | 90 | 33.118 | 55.203 | 26.561 | 1.00 | 0.00 |
| ATOM | 2371 | CB | PRO | 1 | 90 | 32.476 | 57.392 | 24.824 | 1.00 | 0.00 |
| ATOM | 2372 | CG | PRO | 1 | 90 | 32.057 | 58.008 | 23.503 | 1.00 | 0.00 |
| ATOM | 2373 | CD | PRO | 1 | 90 | 31.856 | 56.785 | 22.626 | 1.00 | 0.00 |
| ATOM | 2374 | N | LEU | 1 | 91 | 34.931 | 54.648 | 25.235 | 1.00 | 0.00 |
| ATOM | 2375 | CA | LEU | 1 | 91 | 35.832 | 53.949 | 26.155 | 1.00 | 0.00 |
| ATOM | 2376 | C | LEU | 1 | 91 | 36.278 | 54.857 | 27.292 | 1.00 | 0.00 |
| ATOM | 2377 | O | LEU | 1 | 91 | 35.641 | 55.877 | 27.533 | 1.00 | 0.00 |
| ATOM | 2378 | CB | LEU | 1 | 91 | 37.017 | 53.451 | 25.341 | 1.00 | 0.00 |
| ATOM | 2379 | CG | LEU | 1 | 91 | 37.509 | 52.090 | 25.793 | 1.00 | 0.00 |
| ATOM | 2380 | CD1 | LEU | 1 | 91 | 36.708 | 50.958 | 25.148 | 1.00 | 0.00 |
| ATOM | 2381 | CD2 | LEU | 1 | 91 | 39.017 | 51.976 | 25.618 | 1.00 | 0.00 |
| ATOM | 2382 | H | LEU | 1 | 91 | 35.213 | 54.609 | 24.276 | 1.00 | 0.00 |
| ATOM | 2383 | N | THR | 1 | 92 | 37.313 | 54.529 | 28.041 | 1.00 | 0.00 |
| ATOM | 2384 | CA | THR | 1 | 92 | 37.352 | 55.082 | 29.402 | 1.00 | 0.00 |
| ATOM | 2385 | C | THR | 1 | 92 | 38.730 | 55.454 | 29.921 | 1.00 | 0.00 |
| ATOM | 2386 | O | THR | 1 | 92 | 39.680 | 54.730 | 29.671 | 1.00 | 0.00 |
| ATOM | 2387 | CB | THR | 1 | 92 | 36.650 | 54.028 | 30.260 | 1.00 | 0.00 |
| ATOM | 2388 | OG1 | THR | 1 | 92 | 35.272 | 53.988 | 29.860 | 1.00 | 0.00 |
| ATOM | 2389 | CG2 | THR | 1 | 92 | 36.791 | 54.149 | 31.778 | 1.00 | 0.00 |
| ATOM | 2390 | H | THR | 1 | 92 | 37.999 | 53.026 | 27.759 | 1.00 | 0.00 |
| ATOM | 2391 | HG1 | THR | 1 | 92 | 39.293 | 53.444 | 29.067 | 1.00 | 0.00 |
| ATOM | 2392 | N | ILE | 1 | 93 | 38.844 | 56.591 | 30.614 | 1.00 | 0.00 |
| ATOM | 2393 | CA | ILE | 1 | 93 | 40.191 | 56.965 | 31.058 | 1.00 | 0.00 |
| ATOM | 2394 | C | ILE | 1 | 93 | 40.562 | 56.426 | 32.438 | 1.00 | 0.00 |
| ATOM | 2395 | O | ILE | 1 | 93 | 39.905 | 56.718 | 33.443 | 1.00 | 0.00 |
| ATOM | 2396 | CB | ILE | 1 | 93 | 40.371 | 58.493 | 30.927 | 1.00 | 0.00 |
| ATOM | 2397 | CG1 | ILE | 1 | 93 | 41.779 | 58.953 | 31.322 | 1.00 | 0.00 |
| ATOM | 2398 | CG2 | ILE | 1 | 93 | 39.296 | 59.264 | 31.710 | 1.00 | 0.00 |
| ATOM | 2399 | CD1 | ILE | 1 | 93 | 42.043 | 60.422 | 30.983 | 1.00 | 0.00 |
| ATOM | 2400 | H | ILE | 1 | 93 | 38.046 | 57.149 | 30.825 | 1.00 | 0.00 |
| ATOM | 2401 | N | THR | 1 | 94 | 41.616 | 55.597 | 32.440 | 1.00 | 0.00 |
| ATOM | 2402 | CA | THR | 1 | 94 | 42.106 | 54.953 | 33.663 | 1.00 | 0.00 |
| ATOM | 2403 | C | THR | 1 | 94 | 43.500 | 54.432 | 33.330 | 1.00 | 0.00 |
| ATOM | 2404 | O | THR | 1 | 94 | 43.699 | 54.111 | 32.173 | 1.00 | 0.00 |
| ATOM | 2405 | CB | THR | 1 | 94 | 41.166 | 53.787 | 34.037 | 1.00 | 0.00 |
| ATOM | 2406 | OG1 | THR | 1 | 94 | 39.796 | 54.039 | 33.628 | 1.00 | 0.00 |
| ATOM | 2407 | CG2 | THR | 1 | 94 | 41.227 | 53.511 | 35.540 | 1.00 | 0.00 |
| ATOM | 2408 | H | THR | 1 | 94 | 42.105 | 55.397 | 31.584 | 1.00 | 0.00 |
| ATOM | 2409 | HG1 | THR | 1 | 94 | 39.608 | 54.908 | 33.985 | 1.00 | 0.00 |
| ATOM | 2410 | N | LEU | 1 | 95 | 44.445 | 54.327 | 34.292 | 1.00 | 0.00 |
| ATOM | 2411 | CA | LEU | 1 | 95 | 45.751 | 53.798 | 33.858 | 1.00 | 0.00 |
| ATOM | 2412 | C | LEU | 1 | 95 | 45.631 | 52.347 | 33.387 | 1.00 | 0.00 |
| ATOM | 2413 | O | LEU | 1 | 95 | 46.201 | 51.923 | 32.358 | 1.00 | 0.00 |
| ATOM | 2414 | CB | LEU | 1 | 95 | 46.795 | 53.976 | 34.964 | 1.00 | 0.00 |
| ATOM | 2415 | CG | LEU | 1 | 95 | 48.229 | 53.674 | 34.512 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2416 | CD1 | LEU | 1 | 95 | 48.669 | 54.558 | 33.342 | 1.00 | 0.00 |
| ATOM | 2417 | CD2 | LEU | 1 | 95 | 49.213 | 53.736 | 35.680 | 1.00 | 0.00 |
| ATOM | 2418 | H | LEU | 1 | 95 | 44.312 | 54.664 | 35.217 | 1.00 | 0.00 |
| ATOM | 2419 | N | VAL | 1 | 96 | 44.879 | 51.607 | 34.170 | 1.00 | 0.00 |
| ATOM | 2420 | CA | VAL | 1 | 96 | 44.444 | 50.292 | 33.679 | 1.00 | 0.00 |
| ATOM | 2421 | C | VAL | 1 | 96 | 43.497 | 50.291 | 32.471 | 1.00 | 0.00 |
| ATOM | 2422 | O | VAL | 1 | 96 | 42.812 | 49.325 | 32.139 | 1.00 | 0.00 |
| ATOM | 2423 | CB | VAL | 1 | 96 | 43.881 | 49.451 | 34.835 | 1.00 | 0.00 |
| ATOM | 2424 | CG1 | VAL | 1 | 96 | 44.958 | 49.226 | 35.899 | 1.00 | 0.00 |
| ATOM | 2425 | CG2 | VAL | 1 | 96 | 42.597 | 50.036 | 35.426 | 1.00 | 0.00 |
| ATOM | 2426 | H | VAL | 1 | 96 | 44.568 | 51.975 | 35.042 | 1.00 | 0.00 |
| ATOM | 2427 | N | ARG | 1 | 97 | 43.470 | 51.438 | 31.787 | 1.00 | 0.00 |
| ATOM | 2428 | CA | ARG | 1 | 97 | 42.784 | 51.396 | 30.512 | 1.00 | 0.00 |
| ATOM | 2429 | C | ARG | 1 | 97 | 43.678 | 51.257 | 29.324 | 1.00 | 0.00 |
| ATOM | 2430 | O | ARG | 1 | 97 | 43.400 | 50.425 | 28.473 | 1.00 | 0.00 |
| ATOM | 2431 | CB | ARG | 1 | 97 | 41.808 | 52.538 | 30.335 | 1.00 | 0.00 |
| ATOM | 2432 | CG | ARG | 1 | 97 | 40.455 | 52.056 | 30.825 | 1.00 | 0.00 |
| ATOM | 2433 | CD | ARG | 1 | 97 | 39.958 | 50.912 | 29.954 | 1.00 | 0.00 |
| ATOM | 2434 | NE | ARG | 1 | 97 | 38.651 | 50.485 | 30.421 | 1.00 | 0.00 |
| ATOM | 2435 | CZ | ARG | 1 | 97 | 37.694 | 50.168 | 29.535 | 1.00 | 0.00 |
| ATOM | 2436 | NH1 | ARG | 1 | 97 | 36.459 | 50.024 | 29.991 | 1.00 | 0.00 |
| ATOM | 2437 | NH2 | ARG | 1 | 97 | 37.962 | 50.048 | 28.242 | 1.00 | 0.00 |
| ATOM | 2438 | H | ARG | 1 | 97 | 44.066 | 52.223 | 31.934 | 1.00 | 0.00 |
| ATOM | 2439 | HE | ARG | 1 | 97 | 38.525 | 50.498 | 31.415 | 1.00 | 0.00 |
| ATOM | 2440 | 1HH1 | ARG | 1 | 97 | 35.707 | 49.766 | 29.382 | 1.00 | 0.00 |
| ATOM | 2441 | 2HH1 | ARG | 1 | 97 | 36.283 | 50.158 | 30.968 | 1.00 | 0.00 |
| ATOM | 2442 | 1HH2 | ARG | 1 | 97 | 37.251 | 49.995 | 27.535 | 1.00 | 0.00 |
| ATOM | 2443 | 2HH2 | ARG | 1 | 97 | 38.908 | 50.019 | 27.913 | 1.00 | 0.00 |
| ATOM | 2444 | N | GLU | 1 | 98 | 44.767 | 52.020 | 29.273 | 1.00 | 0.00 |
| ATOM | 2445 | CA | GLU | 1 | 98 | 45.745 | 51.584 | 28.282 | 1.00 | 0.00 |
| ATOM | 2446 | C | GLU | 1 | 98 | 46.451 | 50.311 | 28.713 | 1.00 | 0.00 |
| ATOM | 2447 | O | GLU | 1 | 98 | 46.514 | 49.295 | 28.025 | 1.00 | 0.00 |
| ATOM | 2448 | CB | GLU | 1 | 98 | 46.717 | 52.699 | 27.844 | 1.00 | 0.00 |
| ATOM | 2449 | CG | GLU | 1 | 98 | 47.244 | 53.642 | 28.883 | 1.00 | 0.00 |
| ATOM | 2450 | CD | GLU | 1 | 98 | 46.349 | 54.690 | 29.353 | 1.00 | 0.00 |
| ATOM | 2451 | OE1 | GLU | 1 | 98 | 46.201 | 55.728 | 28.717 | 1.00 | 0.00 |
| ATOM | 2452 | OE2 | GLU | 1 | 98 | 45.717 | 54.475 | 30.373 | 1.00 | 0.00 |
| ATOM | 2453 | H | GLU | 1 | 98 | 44.913 | 52.735 | 29.955 | 1.00 | 0.00 |
| ATOM | 2454 | N | GLU | 1 | 99 | 46.966 | 50.359 | 29.943 | 1.00 | 0.00 |
| ATOM | 2455 | CA | GLU | 1 | 99 | 47.643 | 49.136 | 30.361 | 1.00 | 0.00 |
| ATOM | 2456 | C | GLU | 1 | 99 | 46.782 | 48.071 | 31.020 | 1.00 | 0.00 |
| ATOM | 2457 | O | GLU | 1 | 99 | 47.232 | 47.192 | 31.744 | 1.00 | 0.00 |
| ATOM | 2458 | CB | GLU | 1 | 99 | 48.958 | 49.451 | 31.083 | 1.00 | 0.00 |
| ATOM | 2459 | CG | GLU | 1 | 99 | 50.078 | 48.456 | 30.744 | 1.00 | 0.00 |
| ATOM | 2460 | CD | GLU | 1 | 99 | 50.314 | 48.313 | 29.238 | 1.00 | 0.00 |
| ATOM | 2461 | OE1 | GLU | 1 | 99 | 50.096 | 49.254 | 28.483 | 1.00 | 0.00 |
| ATOM | 2462 | OE2 | GLU | 1 | 99 | 50.689 | 47.237 | 28.790 | 1.00 | 0.00 |
| ATOM | 2463 | H | GLU | 1 | 99 | 46.825 | 51.157 | 30.526 | 1.00 | 0.00 |
| ATOM | 2464 | N | VAL | 1 | 100 | 45.488 | 48.154 | 30.680 | 1.00 | 0.00 |
| ATOM | 2465 | CA | VAL | 1 | 100 | 44.782 | 46.895 | 30.458 | 1.00 | 0.00 |
| ATOM | 2466 | C | VAL | 1 | 100 | 44.096 | 46.924 | 29.098 | 1.00 | 0.00 |
| ATOM | 2467 | O | VAL | 1 | 100 | 44.514 | 46.268 | 28.149 | 1.00 | 0.00 |
| ATOM | 2468 | CB | VAL | 1 | 100 | 43.794 | 46.486 | 31.578 | 1.00 | 0.00 |
| ATOM | 2469 | CG1 | VAL | 1 | 100 | 43.117 | 45.144 | 31.274 | 1.00 | 0.00 |
| ATOM | 2470 | CG2 | VAL | 1 | 100 | 44.458 | 46.398 | 32.952 | 1.00 | 0.00 |
| ATOM | 2471 | H | VAL | 1 | 100 | 45.139 | 48.985 | 30.256 | 1.00 | 0.00 |
| ATOM | 2472 | N | ILE | 1 | 101 | 42.988 | 47.671 | 28.995 | 1.00 | 0.00 |
| ATOM | 2473 | CA | ILE | 1 | 101 | 42.246 | 47.533 | 27.731 | 1.00 | 0.00 |
| ATOM | 2474 | C | ILE | 1 | 101 | 42.178 | 48.764 | 26.820 | 1.00 | 0.00 |
| ATOM | 2475 | O | ILE | 1 | 101 | 41.223 | 49.557 | 26.863 | 1.00 | 0.00 |
| ATOM | 2476 | CB | ILE | 1 | 101 | 40.870 | 46.870 | 27.957 | 1.00 | 0.00 |
| ATOM | 2477 | CG1 | ILE | 1 | 101 | 40.173 | 47.361 | 29.227 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2478 | CG2 | ILE | 1 | 101 | 41.039 | 45.347 | 28.007 | 1.00 | 0.00 |
| ATOM | 2479 | CD1 | ILE | 1 | 101 | 38.814 | 46.694 | 29.457 | 1.00 | 0.00 |
| ATOM | 2480 | H | ILE | 1 | 101 | 42.741 | 48.277 | 29.753 | 1.00 | 0.00 |
| ATOM | 2481 | N | ASP | 1 | 102 | 43.277 | 48.854 | 26.039 | 1.00 | 0.00 |
| ATOM | 2482 | CA | ASP | 1 | 102 | 43.843 | 50.034 | 25.377 | 1.00 | 0.00 |
| ATOM | 2483 | C | ASP | 1 | 102 | 42.955 | 51.086 | 24.775 | 1.00 | 0.00 |
| ATOM | 2484 | O | ASP | 1 | 102 | 41.750 | 50.949 | 24.580 | 1.00 | 0.00 |
| ATOM | 2485 | CB | ASP | 1 | 102 | 44.900 | 49.660 | 24.335 | 1.00 | 0.00 |
| ATOM | 2486 | CG | ASP | 1 | 102 | 46.164 | 49.173 | 24.991 | 1.00 | 0.00 |
| ATOM | 2487 | OD1 | ASP | 1 | 102 | 47.123 | 49.928 | 25.101 | 1.00 | 0.00 |
| ATOM | 2488 | OD2 | ASP | 1 | 102 | 46.203 | 48.023 | 25.393 | 1.00 | 0.00 |
| ATOM | 2489 | H | ASP | 1 | 102 | 43.948 | 48.129 | 26.173 | 1.00 | 0.00 |
| ATOM | 2490 | N | PHE | 1 | 103 | 43.635 | 52.203 | 24.510 | 1.00 | 0.00 |
| ATOM | 2491 | CA | PHE | 1 | 103 | 42.962 | 53.493 | 24.440 | 1.00 | 0.00 |
| ATOM | 2492 | C | PHE | 1 | 103 | 43.031 | 54.203 | 23.091 | 1.00 | 0.00 |
| ATOM | 2493 | O | PHE | 1 | 103 | 43.430 | 53.644 | 22.066 | 1.00 | 0.00 |
| ATOM | 2494 | CB | PHE | 1 | 103 | 43.525 | 54.345 | 25.596 | 1.00 | 0.00 |
| ATOM | 2495 | CG | PHE | 1 | 103 | 44.894 | 54.956 | 25.328 | 1.00 | 0.00 |
| ATOM | 2496 | CD1 | PHE | 1 | 103 | 45.087 | 56.312 | 25.668 | 1.00 | 0.00 |
| ATOM | 2497 | CD2 | PHE | 1 | 103 | 45.946 | 54.201 | 24.759 | 1.00 | 0.00 |
| ATOM | 2498 | CE1 | PHE | 1 | 103 | 46.332 | 56.925 | 25.433 | 1.00 | 0.00 |
| ATOM | 2499 | CE2 | PHE | 1 | 103 | 47.194 | 54.808 | 24.522 | 1.00 | 0.00 |
| ATOM | 2500 | CZ | PHE | 1 | 103 | 47.373 | 56.166 | 24.860 | 1.00 | 0.00 |
| ATOM | 2501 | H | PHE | 1 | 103 | 44.628 | 52.124 | 24.432 | 1.00 | 0.00 |
| ATOM | 2502 | N | SER | 1 | 104 | 42.693 | 55.502 | 23.179 | 1.00 | 0.00 |
| ATOM | 2503 | CA | SER | 1 | 104 | 43.287 | 56.497 | 22.295 | 1.00 | 0.00 |
| ATOM | 2504 | C | SER | 1 | 104 | 43.365 | 57.842 | 23.008 | 1.00 | 0.00 |
| ATOM | 2505 | O | SER | 1 | 104 | 42.884 | 57.980 | 24.137 | 1.00 | 0.00 |
| ATOM | 2506 | CB | SER | 1 | 104 | 42.547 | 56.594 | 20.965 | 1.00 | 0.00 |
| ATOM | 2507 | OG | SER | 1 | 104 | 43.418 | 57.227 | 20.009 | 1.00 | 0.00 |
| ATOM | 2508 | H | SER | 1 | 104 | 42.169 | 55.815 | 23.969 | 1.00 | 0.00 |
| ATOM | 2509 | HG | SER | 1 | 104 | 42.856 | 57.416 | 19.261 | 1.00 | 0.00 |
| ATOM | 2510 | N | LYS | 1 | 105 | 43.994 | 58.822 | 22.328 | 1.00 | 0.00 |
| ATOM | 2511 | CA | LYS | 1 | 105 | 44.148 | 60.159 | 22.922 | 1.00 | 0.00 |
| ATOM | 2512 | C | LYS | 1 | 105 | 42.768 | 60.754 | 23.191 | 1.00 | 0.00 |
| ATOM | 2513 | O | LYS | 1 | 105 | 41.861 | 60.440 | 22.423 | 1.00 | 0.00 |
| ATOM | 2514 | CB | LYS | 1 | 105 | 44.924 | 61.023 | 21.919 | 1.00 | 0.00 |
| ATOM | 2515 | CG | LYS | 1 | 105 | 45.936 | 62.004 | 22.515 | 1.00 | 0.00 |
| ATOM | 2516 | CD | LYS | 1 | 105 | 46.411 | 63.037 | 21.491 | 1.00 | 0.00 |
| ATOM | 2517 | CE | LYS | 1 | 105 | 47.473 | 63.983 | 22.056 | 1.00 | 0.00 |
| ATOM | 2518 | NZ | LYS | 1 | 105 | 47.542 | 65.179 | 21.212 | 1.00 | 0.00 |
| ATOM | 2519 | H | LYS | 1 | 105 | 44.243 | 58.605 | 21.381 | 1.00 | 0.00 |
| ATOM | 2520 | 1HZ | LYS | 1 | 105 | 46.589 | 65.594 | 21.139 | 1.00 | 0.00 |
| ATOM | 2521 | 2HZ | LYS | 1 | 105 | 48.070 | 65.944 | 21.667 | 1.00 | 0.00 |
| ATOM | 2522 | 3HZ | LYS | 1 | 105 | 47.889 | 65.946 | 20.248 | 1.00 | 0.00 |
| ATOM | 2523 | N | PRO | 1 | 106 | 42.606 | 61.571 | 24.269 | 1.00 | 0.00 |
| ATOM | 2524 | CA | PRO | 1 | 106 | 41.329 | 62.259 | 24.543 | 1.00 | 0.00 |
| ATOM | 2525 | C | PRO | 1 | 106 | 40.570 | 62.908 | 23.380 | 1.00 | 0.00 |
| ATOM | 2526 | O | PRO | 1 | 106 | 40.587 | 64.118 | 23.125 | 1.00 | 0.00 |
| ATOM | 2527 | CB | PRO | 1 | 106 | 41.713 | 63.234 | 25.659 | 1.00 | 0.00 |
| ATOM | 2528 | CG | PRO | 1 | 106 | 42.821 | 62.511 | 26.421 | 1.00 | 0.00 |
| ATOM | 2529 | CD | PRO | 1 | 106 | 43.600 | 61.817 | 25.309 | 1.00 | 0.00 |
| ATOM | 2530 | N | PHE | 1 | 107 | 39.825 | 62.029 | 22.692 | 1.00 | 0.00 |
| ATOM | 2531 | CA | PHE | 1 | 107 | 39.071 | 62.548 | 21.560 | 1.00 | 0.00 |
| ATOM | 2532 | C | PHE | 1 | 107 | 37.603 | 62.778 | 21.831 | 1.00 | 0.00 |
| ATOM | 2533 | O | PHE | 1 | 107 | 36.963 | 63.606 | 21.188 | 1.00 | 0.00 |
| ATOM | 2534 | CB | PHE | 1 | 107 | 39.225 | 61.657 | 20.317 | 1.00 | 0.00 |
| ATOM | 2535 | CG | PHE | 1 | 107 | 40.638 | 61.658 | 19.771 | 1.00 | 0.00 |
| ATOM | 2536 | CD1 | PHE | 1 | 107 | 41.312 | 62.879 | 19.533 | 1.00 | 0.00 |
| ATOM | 2537 | CD2 | PHE | 1 | 107 | 41.258 | 60.421 | 19.485 | 1.00 | 0.00 |
| ATOM | 2538 | CE1 | PHE | 1 | 107 | 42.617 | 62.861 | 19.004 | 1.00 | 0.00 |
| ATOM | 2539 | CE2 | PHE | 1 | 107 | 42.563 | 60.400 | 18.956 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2540 | CZ | PHE | 1 | 107 | 43.228 | 61.622 | 18.718 | 1.00 | 0.00 |
| ATOM | 2541 | H | PHE | 1 | 107 | 39.946 | 61.055 | 22.910 | 1.00 | 0.00 |
| ATOM | 2542 | N | MET | 1 | 108 | 37.060 | 61.980 | 22.765 | 1.00 | 0.00 |
| ATOM | 2543 | CA | MET | 1 | 108 | 35.601 | 62.083 | 22.856 | 1.00 | 0.00 |
| ATOM | 2544 | C | MET | 1 | 108 | 34.980 | 63.079 | 23.816 | 1.00 | 0.00 |
| ATOM | 2545 | O | MET | 1 | 108 | 34.000 | 63.764 | 23.506 | 1.00 | 0.00 |
| ATOM | 2546 | CB | MET | 1 | 108 | 34.945 | 60.714 | 22.942 | 1.00 | 0.00 |
| ATOM | 2547 | CG | MET | 1 | 108 | 34.020 | 60.522 | 21.737 | 1.00 | 0.00 |
| ATOM | 2548 | SD | MET | 1 | 108 | 34.885 | 60.418 | 20.156 | 1.00 | 0.00 |
| ATOM | 2549 | CE | MET | 1 | 108 | 34.587 | 62.089 | 19.552 | 1.00 | 0.00 |
| ATOM | 2550 | H | MET | 1 | 108 | 37.613 | 61.351 | 23.313 | 1.00 | 0.00 |
| ATOM | 2551 | N | SER | 1 | 109 | 35.622 | 63.173 | 24.991 | 1.00 | 0.00 |
| ATOM | 2552 | CA | SER | 1 | 109 | 35.476 | 64.400 | 25.779 | 1.00 | 0.00 |
| ATOM | 2553 | C | SER | 1 | 109 | 34.039 | 64.723 | 26.216 | 1.00 | 0.00 |
| ATOM | 2554 | O | SER | 1 | 109 | 33.155 | 63.872 | 26.105 | 1.00 | 0.00 |
| ATOM | 2555 | CB | SER | 1 | 109 | 36.200 | 65.531 | 25.027 | 1.00 | 0.00 |
| ATOM | 2556 | OG | SER | 1 | 109 | 37.214 | 64.984 | 24.141 | 1.00 | 0.00 |
| ATOM | 2557 | H | SER | 1 | 109 | 36.293 | 62.475 | 25.227 | 1.00 | 0.00 |
| ATOM | 2558 | HG | SER | 1 | 109 | 37.580 | 65.723 | 23.638 | 1.00 | 0.00 |
| ATOM | 2559 | N | LEU | 1 | 110 | 33.848 | 65.963 | 26.761 | 1.00 | 0.00 |
| ATOM | 2560 | CA | LEU | 1 | 110 | 32.599 | 66.482 | 27.373 | 1.00 | 0.00 |
| ATOM | 2561 | C | LEU | 1 | 110 | 32.394 | 65.945 | 28.789 | 1.00 | 0.00 |
| ATOM | 2562 | O | LEU | 1 | 110 | 32.668 | 64.769 | 29.047 | 1.00 | 0.00 |
| ATOM | 2563 | CB | LEU | 1 | 110 | 31.372 | 66.294 | 26.452 | 1.00 | 0.00 |
| ATOM | 2564 | CG | LEU | 1 | 110 | 30.204 | 67.286 | 26.600 | 1.00 | 0.00 |
| ATOM | 2565 | CD1 | LEU | 1 | 110 | 29.270 | 66.978 | 27.772 | 1.00 | 0.00 |
| ATOM | 2566 | CD2 | LEU | 1 | 110 | 30.679 | 68.740 | 26.609 | 1.00 | 0.00 |
| ATOM | 2567 | H | LEU | 1 | 110 | 34.667 | 66.532 | 26.874 | 1.00 | 0.00 |
| ATOM | 2568 | N | GLY | 1 | 111 | 32.002 | 66.827 | 29.726 | 1.00 | 0.00 |
| ATOM | 2569 | CA | GLY | 1 | 111 | 32.226 | 66.455 | 31.133 | 1.00 | 0.00 |
| ATOM | 2570 | C | GLY | 1 | 111 | 30.992 | 66.172 | 31.976 | 1.00 | 0.00 |
| ATOM | 2571 | O | GLY | 1 | 111 | 29.881 | 66.610 | 31.642 | 1.00 | 0.00 |
| ATOM | 2572 | H | GLY | 1 | 111 | 31.732 | 67.749 | 29.447 | 1.00 | 0.00 |
| ATOM | 2573 | N | ILE | 1 | 112 | 31.236 | 65.419 | 33.071 | 1.00 | 0.00 |
| ATOM | 2574 | CA | ILE | 1 | 112 | 30.184 | 65.069 | 34.029 | 1.00 | 0.00 |
| ATOM | 2575 | C | ILE | 1 | 112 | 29.338 | 66.275 | 34.398 | 1.00 | 0.00 |
| ATOM | 2576 | O | ILE | 1 | 112 | 29.773 | 67.281 | 34.962 | 1.00 | 0.00 |
| ATOM | 2577 | CB | ILE | 1 | 112 | 30.756 | 64.341 | 35.262 | 1.00 | 0.00 |
| ATOM | 2578 | CG1 | ILE | 1 | 112 | 29.071 | 63.816 | 36.202 | 1.00 | 0.00 |
| ATOM | 2579 | CG2 | ILE | 1 | 112 | 31.706 | 65.229 | 36.057 | 1.00 | 0.00 |
| ATOM | 2580 | CD1 | ILE | 1 | 112 | 28.862 | 62.664 | 35.619 | 1.00 | 0.00 |
| ATOM | 2581 | H | ILE | 1 | 112 | 32.204 | 65.258 | 33.247 | 1.00 | 0.00 |
| ATOM | 2582 | N | SER | 1 | 113 | 28.105 | 66.162 | 33.901 | 1.00 | 0.00 |
| ATOM | 2583 | CA | SER | 1 | 113 | 27.215 | 67.317 | 33.849 | 1.00 | 0.00 |
| ATOM | 2584 | C | SER | 1 | 113 | 26.551 | 67.591 | 35.194 | 1.00 | 0.00 |
| ATOM | 2585 | O | SER | 1 | 113 | 25.470 | 67.108 | 35.552 | 1.00 | 0.00 |
| ATOM | 2586 | CB | SER | 1 | 113 | 26.254 | 67.138 | 32.663 | 1.00 | 0.00 |
| ATOM | 2587 | OG | SER | 1 | 113 | 26.985 | 66.790 | 31.454 | 1.00 | 0.00 |
| ATOM | 2588 | H | SER | 1 | 113 | 27.810 | 65.269 | 33.565 | 1.00 | 0.00 |
| ATOM | 2589 | HG | SER | 1 | 113 | 26.644 | 67.436 | 30.833 | 1.00 | 0.00 |
| ATOM | 2590 | N | ILE | 1 | 114 | 27.351 | 68.334 | 35.973 | 1.00 | 0.00 |
| ATOM | 2591 | CA | ILE | 1 | 114 | 27.115 | 68.453 | 37.404 | 1.00 | 0.00 |
| ATOM | 2592 | C | ILE | 1 | 114 | 25.996 | 69.422 | 37.707 | 1.00 | 0.00 |
| ATOM | 2593 | O | ILE | 1 | 114 | 26.044 | 70.593 | 37.326 | 1.00 | 0.00 |
| ATOM | 2594 | CB | ILE | 1 | 114 | 28.425 | 68.844 | 38.134 | 1.00 | 0.00 |
| ATOM | 2595 | CG1 | ILE | 1 | 114 | 29.492 | 67.765 | 37.953 | 1.00 | 0.00 |
| ATOM | 2596 | CG2 | ILE | 1 | 114 | 28.229 | 69.048 | 39.688 | 1.00 | 0.00 |
| ATOM | 2597 | CD1 | ILE | 1 | 114 | 30.785 | 68.023 | 38.733 | 1.00 | 0.00 |
| ATOM | 2598 | H | ILE | 1 | 114 | 28.170 | 68.718 | 35.545 | 1.00 | 0.00 |
| ATOM | 2599 | N | MET | 1 | 115 | 25.041 | 68.859 | 38.470 | 1.00 | 0.00 |
| ATOM | 2600 | CA | MET | 1 | 115 | 23.955 | 69.635 | 39.063 | 1.00 | 0.00 |
| ATOM | 2601 | C | MET | 1 | 115 | 22.349 | 69.972 | 38.081 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2602 | O | MET | 1 | 115 | 22.597 | 71.113 | 37.700 | 1.00 | 0.00 |
| ATOM | 2603 | CB | MET | 1 | 115 | 24.448 | 70.834 | 39.814 | 1.00 | 0.00 |
| ATOM | 2604 | CG | MET | 1 | 115 | 25.420 | 70.678 | 40.974 | 1.00 | 0.00 |
| ATOM | 2605 | SD | MET | 1 | 115 | 24.768 | 69.687 | 42.319 | 1.00 | 0.00 |
| ATOM | 2606 | CE | MET | 1 | 115 | 26.365 | 69.226 | 43.009 | 1.00 | 0.00 |
| ATOM | 2607 | H | MET | 1 | 115 | 25.011 | 67.859 | 38.522 | 1.00 | 0.00 |
| ATOM | 2608 | N | ILE | 1 | 116 | 22.144 | 68.885 | 37.687 | 1.00 | 0.00 |
| ATOM | 2609 | CA | ILE | 1 | 116 | 20.943 | 69.162 | 36.883 | 1.00 | 0.00 |
| ATOM | 2610 | C | ILE | 1 | 116 | 19.697 | 69.284 | 37.748 | 1.00 | 0.00 |
| ATOM | 2611 | O | ILE | 1 | 116 | 19.548 | 68.524 | 38.693 | 1.00 | 0.00 |
| ATOM | 2612 | CB | ILE | 1 | 116 | 20.782 | 68.225 | 35.672 | 1.00 | 0.00 |
| ATOM | 2613 | CG1 | ILE | 1 | 116 | 20.144 | 66.865 | 35.951 | 1.00 | 0.00 |
| ATOM | 2614 | CG2 | ILE | 1 | 116 | 22.148 | 68.077 | 34.994 | 1.00 | 0.00 |
| ATOM | 2615 | CD1 | ILE | 1 | 116 | 18.641 | 66.824 | 35.656 | 1.00 | 0.00 |
| ATOM | 2616 | H | ILE | 1 | 116 | 22.388 | 67.980 | 38.046 | 1.00 | 0.00 |
| ATOM | 2617 | N | LYS | 1 | 117 | 18.928 | 70.359 | 37.504 | 1.00 | 0.00 |
| ATOM | 2618 | CA | LYS | 1 | 117 | 18.521 | 71.127 | 38.682 | 1.00 | 0.00 |
| ATOM | 2619 | C | LYS | 1 | 117 | 17.533 | 72.242 | 38.336 | 1.00 | 0.00 |
| ATOM | 2620 | O | LYS | 1 | 117 | 16.677 | 72.088 | 37,461 | 1.00 | 0.00 |
| ATOM | 2621 | CB | LYS | 1 | 117 | 19.805 | 71.583 | 39.386 | 1.00 | 0.00 |
| ATOM | 2622 | CG | LYS | 1 | 117 | 19.875 | 71.983 | 40.857 | 1.00 | 0.00 |
| ATOM | 2623 | CD | LYS | 1 | 117 | 21.337 | 72.179 | 41.275 | 1.00 | 0.00 |
| ATOM | 2624 | CE | LYS | 1 | 117 | 22.134 | 73.324 | 40.614 | 1.00 | 0.00 |
| ATOM | 2625 | NZ | LYS | 1 | 117 | 22.274 | 73.193 | 39.160 | 1.00 | 0.00 |
| ATOM | 2626 | H | LYS | 1 | 117 | 18.953 | 70.808 | 36.613 | 1.00 | 0.00 |
| ATOM | 2627 | 1HZ | LYS | 1 | 117 | 21.344 | 73.357 | 38.726 | 1.00 | 0.00 |
| ATOM | 2628 | 2HZ | LYS | 1 | 117 | 22.961 | 73.828 | 38.721 | 1.00 | 0.00 |
| ATOM | 2629 | 3HZ | LYS | 1 | 117 | 22.537 | 72.236 | 38.889 | 1.00 | 0.00 |
| ATOM | 2630 | N | LYS | 1 | 118 | 17.589 | 73.353 | 39.093 | 1.00 | 0.00 |
| ATOM | 2631 | CA | LYS | 1 | 118 | 16.634 | 74.456 | 38.972 | 1.00 | 0.00 |
| ATOM | 2632 | C | LYS | 1 | 118 | 17.295 | 75.828 | 39.070 | 1.00 | 0.00 |
| ATOM | 2633 | O | LYS | 1 | 118 | 17.653 | 76.355 | 40.130 | 1.00 | 0.00 |
| ATOM | 2634 | CB | LYS | 1 | 118 | 15.495 | 74.326 | 39.992 | 1.00 | 0.00 |
| ATOM | 2635 | CG | LYS | 1 | 118 | 14.499 | 73.228 | 39.610 | 1.00 | 0.00 |
| ATOM | 2636 | CD | LYS | 1 | 118 | 13.760 | 73.556 | 38.307 | 1.00 | 0.00 |
| ATOM | 2637 | CE | LYS | 1 | 118 | 13.209 | 72.322 | 37.589 | 1.00 | 0.00 |
| ATOM | 2638 | NZ | LYS | 1 | 118 | 14.309 | 71.565 | 36.995 | 1.00 | 0.00 |
| ATOM | 2639 | H | LYS | 1 | 118 | 18.395 | 73.585 | 39.636 | 1.00 | 0.00 |
| ATOM | 2640 | 1HZ | LYS | 1 | 118 | 15.020 | 71.355 | 37.723 | 1.00 | 0.00 |
| ATOM | 2641 | 2HZ | LYS | 1 | 118 | 13.947 | 70.703 | 36.560 | 1.00 | 0.00 |
| ATOM | 2642 | 3HZ | LYS | 1 | 118 | 14.819 | 72.120 | 36.286 | 1.00 | 0.00 |
| ATOM | 2643 | N | PRO | 1 | 119 | 17.416 | 76.435 | 37.865 | 1.00 | 0.00 |
| ATOM | 2644 | CA | PRO | 1 | 119 | 18.069 | 77.745 | 37.769 | 1.00 | 0.00 |
| ATOM | 2645 | C | PRO | 1 | 119 | 17.178 | 78.836 | 38.354 | 1.00 | 0.00 |
| ATOM | 2646 | O | PRO | 1 | 119 | 16.284 | 78.580 | 39.163 | 1.00 | 0.00 |
| ATOM | 2647 | CB | PRO | 1 | 119 | 18.298 | 77.861 | 36.254 | 1.00 | 0.00 |
| ATOM | 2648 | CG | PRO | 1 | 119 | 17.134 | 77.105 | 35.619 | 1.00 | 0.00 |
| ATOM | 2649 | CD | PRO | 1 | 119 | 16.961 | 75.931 | 36.571 | 1.00 | 0.00 |
| ATOM | 2650 | N | GLY | 1 | 120 | 17.432 | 80.054 | 37.882 | 1.00 | 0.00 |
| ATOM | 2651 | CA | GLY | 1 | 120 | 16.488 | 81.150 | 38.077 | 1.00 | 0.00 |
| ATOM | 2652 | C | GLY | 1 | 120 | 16.735 | 82.074 | 36.911 | 1.00 | 0.00 |
| ATOM | 2653 | O | GLY | 1 | 120 | 17.735 | 81.888 | 36.224 | 1.00 | 0.00 |
| ATOM | 2654 | H | GLY | 1 | 120 | 18.259 | 80.180 | 37.332 | 1.00 | 0.00 |
| ATOM | 2655 | N | LYS | 1 | 121 | 15.845 | 83.051 | 36.675 | 1.00 | 0.00 |
| ATOM | 2656 | CA | LYS | 1 | 121 | 16.255 | 84.015 | 35.645 | 1.00 | 0.00 |
| ATOM | 2657 | C | LYS | 1 | 121 | 17.029 | 85.195 | 36.208 | 1.00 | 0.00 |
| ATOM | 2658 | O | LYS | 1 | 121 | 16.769 | 86.365 | 35.935 | 1.00 | 0.00 |
| ATOM | 2659 | CB | LYS | 1 | 121 | 15.091 | 84.462 | 34.747 | 1.00 | 0.00 |
| ATOM | 2660 | CG | LYS | 1 | 121 | 14.642 | 82.367 | 33.771 | 1.00 | 0.00 |
| ATOM | 2661 | CD | LYS | 1 | 121 | 13.800 | 83.891 | 32.598 | 1.00 | 0.00 |
| ATOM | 2662 | CE | LYS | 1 | 121 | 13.424 | 82.780 | 31.608 | 1.00 | 0.00 |
| ATOM | 2663 | NZ | LYS | 1 | 121 | 12.838 | 83.335 | 30.376 | 1.00 | 0.00 |

```
ATOM   2664  H     LYS  1     121     15.050  83.256  37.247  1.00  0.00
ATOM   2665  1HZ   LYS  1     121     13.498  84.009  29.945  1.00  0.00
ATOM   2666  2HZ   LYS  1     121     12.672  82.574  29.690  1.00  0.00
ATOM   2667  3HZ   LYS  1     121     11.937  83.806  30.577  1.00  0.00
ATOM   2668  N     SER  1     122     18.006  84.796  37.037  1.00  0.00
ATOM   2669  CA    SER  1     122     18.929  85.779  37.576  1.00  0.00
ATOM   2670  C     SER  1     122     20.170  85.797  36.716  1.00  0.00
ATOM   2671  O     SER  1     122     20.911  84.822  36.614  1.00  0.00
ATOM   2672  CB    SER  1     122     19.240  85.459  39.038  1.00  0.00
ATOM   2673  OG    SER  1     122     18.913  84.087  39.351  1.00  0.00
ATOM   2674  H     SER  1     122     18.239  83.835  37.160  1.00  0.00
ATOM   2675  HG    SER  1     122     19.094  84.033  40.291  1.00  0.00
ATOM   2676  N     LYS  1     123     20.305  86.945  36.029  1.00  0.00
ATOM   2677  CA    LYS  1     123     21.359  87.150  35.030  1.00  0.00
ATOM   2678  C     LYS  1     123     21.498  86.028  33.997  1.00  0.00
ATOM   2679  O     LYS  1     123     22.276  85.091  34.134  1.00  0.00
ATOM   2680  CB    LYS  1     123     22.687  87.523  35.721  1.00  0.00
ATOM   2681  CG    LYS  1     123     23.643  88.378  34.873  1.00  0.00
ATOM   2682  CD    LYS  1     123     24.364  87.593  33.778  1.00  0.00
ATOM   2683  CE    LYS  1     123     24.968  88.459  32.677  1.00  0.00
ATOM   2684  NZ    LYS  1     123     25.421  87.588  31.593  1.00  0.00
ATOM   2685  H     LYS  1     123     19.616  87.646  36.209  1.00  0.00
ATOM   2686  1HZ   LYS  1     123     24.815  86.746  31.488  1.00  0.00
ATOM   2687  2HZ   LYS  1     123     25.454  88.106  30.692  1.00  0.00
ATOM   2688  3HZ   LYS  1     123     26.400  87.278  31.732  1.00  0.00
ATOM   2689  N     PRO  1     124     20.686  86.146  32.924  1.00  0.00
ATOM   2690  CA    PRO  1     124     20.755  85.140  31.858  1.00  0.00
ATOM   2691  C     PRO  1     124     22.033  85.301  31.025  1.00  0.00
ATOM   2692  O     PRO  1     124     22.806  86.237  31.204  1.00  0.00
ATOM   2693  CB    PRO  1     124     19.478  85.422  31.076  1.00  0.00
ATOM   2694  CG    PRO  1     124     19.244  86.925  31.236  1.00  0.00
ATOM   2695  CD    PRO  1     124     19.697  87.188  32.667  1.00  0.00
ATOM   2696  N     GLY  1     125     22.187  84.360  30.074  1.00  0.00
ATOM   2697  CA    GLY  1     125     23.347  84.355  29.175  1.00  0.00
ATOM   2698  C     GLY  1     125     23.793  85.683  28.574  1.00  0.00
ATOM   2699  O     GLY  1     125     23.049  86.832  27.048  1.00  0.00
ATOM   2700  H     GLY  1     125     21.554  83.583  30.097  1.00  0.00
ATOM   2701  N     GLY  1     126     25.051  86.015  28.895  1.00  0.00
ATOM   2702  CA    GLY  1     126     25.720  87.148  28.266  1.00  0.00
ATOM   2703  C     GLY  1     126     26.936  87.561  29.083  1.00  0.00
ATOM   2704  1OCT  GLY  1     126     26.894  88.596  29.734  1.00  0.00
ATOM   2705  2OCT  GLY  1     126     27.923  86.836  29.109  1.00  0.00
ATOM   2706  H     GLY  1     126     25.528  85.446  29.564  1.00  0.00
END
```

**TABLE 4**

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| REMARK | 1 | Ka | Receptor | | (GluR6) | Model | of | the | glutamate | binding site |
| ATOM | 1 | N | SER | 1 | 427 | 47.092 | 43.380 | 10.501 | 1.00 | 0.00 |
| ATOM | 2 | CA | SER | 1 | 427 | 47.313 | 44.694 | 11.108 | 1.00 | 0.00 |
| ATOM | 3 | C | SER | 1 | 427 | 45.964 | 45.140 | 11.604 | 1.00 | 0.00 |
| ATOM | 4 | O | SER | 1 | 427 | 45.123 | 44.290 | 11.885 | 1.00 | 0.00 |
| ATOM | 5 | CB | SER | 1 | 427 | 47.842 | 45.643 | 10.037 | 1.00 | 0.00 |
| ATOM | 6 | OG | SER | 1 | 427 | 48.684 | 44.947 | 9.101 | 1.00 | 0.00 |
| ATOM | 7 | 1HT | SER | 1 | 427 | 46.213 | 43.433 | 9.943 | 1.00 | 0.00 |
| ATOM | 8 | 2HT | SER | 1 | 427 | 47.904 | 43.154 | 9.893 | 1.00 | 0.00 |
| ATOM | 9 | 3HT | SER | 1 | 427 | 46.929 | 42.671 | 11.242 | 1.00 | 0.00 |
| ATOM | 10 | HG | SER | 1 | 427 | 49.148 | 45.651 | 8.645 | 1.00 | 0.00 |
| ATOM | 11 | N | LEU | 1 | 428 | 45.730 | 46.468 | 11.567 | 1.00 | 0.00 |
| ATOM | 12 | CA | LEU | 1 | 428 | 44.377 | 46.910 | 11.212 | 1.00 | 0.00 |
| ATOM | 13 | C | LEU | 1 | 428 | 43.950 | 46.209 | 9.927 | 1.00 | 0.00 |
| ATOM | 14 | O | LEU | 1 | 428 | 44.508 | 46.464 | 8.856 | 1.00 | 0.00 |
| ATOM | 15 | CB | LEU | 1 | 428 | 44.392 | 48.424 | 11.000 | 1.00 | 0.00 |
| ATOM | 16 | CG | LEU | 1 | 428 | 43.000 | 49.039 | 10.883 | 1.00 | 0.00 |
| ATOM | 17 | CD1 | LEU | 1 | 428 | 42.321 | 49.089 | 12.246 | 1.00 | 0.00 |
| ATOM | 18 | CD2 | LEU | 1 | 428 | 43.023 | 50.409 | 10.208 | 1.00 | 0.00 |
| ATOM | 19 | H | LEU | 1 | 428 | 46.469 | 47.135 | 11.668 | 1.00 | 0.00 |
| ATOM | 20 | N | SER | 1 | 429 | 43.051 | 45.242 | 10.080 | 1.00 | 0.00 |
| ATOM | 21 | CA | SER | 1 | 429 | 42.860 | 44.429 | 8.892 | 1.00 | 0.00 |
| ATOM | 22 | C | SER | 1 | 429 | 41.538 | 44.706 | 8.197 | 1.00 | 0.00 |
| ATOM | 23 | O | SER | 1 | 429 | 40.916 | 45.753 | 8.386 | 1.00 | 0.00 |
| ATOM | 24 | CB | SER | 1 | 429 | 43.170 | 42.962 | 9.222 | 1.00 | 0.00 |
| ATOM | 25 | OG | SER | 1 | 429 | 44.547 | 42.831 | 9.655 | 1.00 | 0.00 |
| ATOM | 26 | H | SER | 1 | 429 | 42.584 | 45.049 | 10.943 | 1.00 | 0.00 |
| ATOM | 27 | HG | SER | 1 | 429 | 44.427 | 42.991 | 10.602 | 1.00 | 0.00 |
| ATOM | 28 | N | ASN | 1 | 430 | 41.125 | 43.779 | 7.312 | 1.00 | 0.00 |
| ATOM | 29 | CA | ASN | 1 | 430 | 39.849 | 44.095 | 6.658 | 1.00 | 0.00 |
| ATOM | 30 | C | ASN | 1 | 430 | 38.637 | 44.024 | 7.583 | 1.00 | 0.00 |
| ATOM | 31 | O | ASN | 1 | 430 | 37.638 | 44.732 | 7.414 | 1.00 | 0.00 |
| ATOM | 32 | CB | ASN | 1 | 430 | 39.640 | 43.257 | 5.395 | 1.00 | 0.00 |
| ATOM | 33 | CG | ASN | 1 | 430 | 38.943 | 44.073 | 4.312 | 1.00 | 0.00 |
| ATOM | 34 | OD1 | ASN | 1 | 430 | 39.439 | 44.214 | 3.200 | 1.00 | 0.00 |
| ATOM | 35 | ND2 | ASN | 1 | 430 | 37.747 | 44.566 | 4.651 | 1.00 | 0.00 |
| ATOM | 36 | H | ASN | 1 | 430 | 41.572 | 42.897 | 7.187 | 1.00 | 0.00 |
| ATOM | 37 | 1HD2 | ASN | 1 | 430 | 37.265 | 45.082 | 3.942 | 1.00 | 0.00 |
| ATOM | 38 | 2HD2 | ASN | 1 | 430 | 37.327 | 44.425 | 5.543 | 1.00 | 0.00 |
| ATOM | 39 | N | ARG | 1 | 431 | 38.797 | 43.145 | 8.581 | 1.00 | 0.00 |
| ATOM | 40 | CA | ARG | 1 | 431 | 37.936 | 43.225 | 9.753 | 1.00 | 0.00 |
| ATOM | 41 | C | ARG | 1 | 431 | 38.722 | 43.986 | 10.797 | 1.00 | 0.00 |
| ATOM | 42 | O | ARG | 1 | 431 | 39.945 | 43.851 | 10.860 | 1.00 | 0.00 |
| ATOM | 43 | CB | ARG | 1 | 431 | 37.594 | 41.811 | 10.228 | 1.00 | 0.00 |
| ATOM | 44 | CG | ARG | 1 | 431 | 37.175 | 40.866 | 9.091 | 1.00 | 0.00 |
| ATOM | 45 | CD | ARG | 1 | 431 | 35.754 | 41.036 | 8.536 | 1.00 | 0.00 |
| ATOM | 46 | NE | ARG | 1 | 431 | 35.460 | 42.390 | 8.059 | 1.00 | 0.00 |
| ATOM | 47 | CZ | ARG | 1 | 431 | 34.254 | 42.935 | 8.318 | 1.00 | 0.00 |
| ATOM | 48 | NH1 | ARG | 1 | 431 | 33.935 | 44.114 | 7.798 | 1.00 | 0.00 |
| ATOM | 49 | NH2 | ARG | 1 | 431 | 33.382 | 42.298 | 9.083 | 1.00 | 0.00 |
| ATOM | 50 | H | ARG | 1 | 431 | 39.688 | 42.724 | 8.724 | 1.00 | 0.00 |
| ATOM | 51 | HE | ARG | 1 | 431 | 36.122 | 42.928 | 7.537 | 1.00 | 0.00 |
| ATOM | 52 | 1HH1 | ARG | 1 | 431 | 33.070 | 44.551 | 8.075 | 1.00 | 0.00 |
| ATOM | 53 | 2HH1 | ARG | 1 | 431 | 34.494 | 44.604 | 7.142 | 1.00 | 0.00 |
| ATOM | 54 | 1HH2 | ARG | 1 | 431 | 32.490 | 42.730 | 9.233 | 1.00 | 0.00 |
| ATOM | 55 | 2HH2 | ARG | 1 | 431 | 33.596 | 41.411 | 9.489 | 1.00 | 0.00 |
| ATOM | 56 | N | SER | 1 | 432 | 37.995 | 44.833 | 11.548 | 1.00 | 0.00 |
| ATOM | 57 | CA | SER | 1 | 432 | 38.563 | 45.819 | 12.483 | 1.00 | 0.00 |
| ATOM | 58 | C | SER | 1 | 432 | 37.449 | 46.706 | 13.009 | 1.00 | 0.00 |
| ATOM | 59 | O | SER | 1 | 432 | 37.086 | 47.703 | 12.386 | 1.00 | 0.00 |
| ATOM | 60 | CB | SER | 1 | 432 | 39.626 | 46.690 | 11.808 | 1.00 | 0.00 |
| ATOM | 61 | OG | SER | 1 | 432 | 39.308 | 46.857 | 10.411 | 1.00 | 0.00 |
| ATOM | 62 | H | SER | 1 | 432 | 36.999 | 44.754 | 11.478 | 1.00 | 0.00 |
| ATOM | 63 | HG | SER | 1 | 432 | 39.842 | 46.205 | 9.949 | 1.00 | 0.00 |
| ATOM | 64 | N | LEU | 1 | 433 | 36.848 | 46.204 | 14.083 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 65 | CA | LEU | 1 | 433 | 35.475 | 46.479 | 14.507 | 1.00 | 0.00 |
| ATOM | 66 | C | LEU | 1 | 433 | 35.300 | 47.726 | 15.388 | 1.00 | 0.00 |
| ATOM | 67 | O | LEU | 1 | 433 | 36.128 | 48.636 | 15.437 | 1.00 | 0.00 |
| ATOM | 68 | CB | LEU | 1 | 433 | 34.979 | 45.242 | 15.281 | 1.00 | 0.00 |
| ATOM | 69 | CG | LEU | 1 | 433 | 34.645 | 43.890 | 14.636 | 1.00 | 0.00 |
| ATOM | 70 | CD1 | LEU | 1 | 433 | 35.669 | 43.315 | 13.655 | 1.00 | 0.00 |
| ATOM | 71 | CD2 | LEU | 1 | 433 | 34.369 | 42.885 | 15.756 | 1.00 | 0.00 |
| ATOM | 72 | H | LEU | 1 | 433 | 37.387 | 45.506 | 14.551 | 1.00 | 0.00 |
| ATOM | 73 | N | ILE | 1 | 434 | 34.200 | 47.654 | 16.179 | 1.00 | 0.00 |
| ATOM | 74 | CA | ILE | 1 | 434 | 33.966 | 48.378 | 17.434 | 1.00 | 0.00 |
| ATOM | 75 | C | ILE | 1 | 434 | 32.965 | 47.592 | 18.279 | 1.00 | 0.00 |
| ATOM | 76 | O | ILE | 1 | 434 | 31.998 | 47.052 | 17.751 | 1.00 | 0.00 |
| ATOM | 77 | CB | ILE | 1 | 434 | 33.468 | 49.813 | 17.148 | 1.00 | 0.00 |
| ATOM | 78 | CG1 | ILE | 1 | 434 | 32.932 | 50.606 | 18.345 | 1.00 | 0.00 |
| ATOM | 79 | CG2 | ILE | 1 | 434 | 32.402 | 49.786 | 16.081 | 1.00 | 0.00 |
| ATOM | 80 | CD1 | ILE | 1 | 434 | 32.194 | 51.873 | 17.901 | 1.00 | 0.00 |
| ATOM | 81 | H | ILE | 1 | 434 | 33.481 | 46.999 | 15.954 | 1.00 | 0.00 |
| ATOM | 82 | N | VAL | 1 | 435 | 33.208 | 47.608 | 19.594 | 1.00 | 0.00 |
| ATOM | 83 | CA | VAL | 1 | 435 | 32.100 | 47.249 | 20.477 | 1.00 | 0.00 |
| ATOM | 84 | C | VAL | 1 | 435 | 31.412 | 48.471 | 21.067 | 1.00 | 0.00 |
| ATOM | 85 | O | VAL | 1 | 435 | 32.065 | 49.397 | 21.577 | 1.00 | 0.00 |
| ATOM | 86 | CB | VAL | 1 | 435 | 32.553 | 46.274 | 21.579 | 1.00 | 0.00 |
| ATOM | 87 | CG1 | VAL | 1 | 435 | 32.893 | 44.913 | 20.976 | 1.00 | 0.00 |
| ATOM | 88 | CG2 | VAL | 1 | 435 | 33.712 | 46.812 | 22.427 | 1.00 | 0.00 |
| ATOM | 89 | H | VAL | 1 | 435 | 34.125 | 47.841 | 19.922 | 1.00 | 0.00 |
| ATOM | 90 | N | THR | 1 | 436 | 30.076 | 48.467 | 20.979 | 1.00 | 0.00 |
| ATOM | 91 | CA | THR | 1 | 436 | 29.280 | 49.491 | 21.657 | 1.00 | 0.00 |
| ATOM | 92 | C | THR | 1 | 436 | 27.861 | 49.028 | 21.912 | 1.00 | 0.00 |
| ATOM | 93 | O | THR | 1 | 436 | 27.220 | 48.384 | 21.080 | 1.00 | 0.00 |
| ATOM | 94 | CB | THR | 1 | 436 | 29.304 | 50.824 | 20.890 | 1.00 | 0.00 |
| ATOM | 95 | OG1 | THR | 1 | 436 | 28.953 | 51.933 | 21.749 | 1.00 | 0.00 |
| ATOM | 96 | CG2 | THR | 1 | 436 | 28.503 | 50.829 | 19.584 | 1.00 | 0.00 |
| ATOM | 97 | H | THR | 1 | 436 | 29.645 | 47.865 | 20.309 | 1.00 | 0.00 |
| ATOM | 98 | HG1 | THR | 1 | 436 | 28.012 | 51.865 | 21.923 | 1.00 | 0.00 |
| ATOM | 99 | N | THR | 1 | 437 | 27.397 | 49.365 | 23.113 | 1.00 | 0.00 |
| ATOM | 100 | CA | THR | 1 | 437 | 26.169 | 48.695 | 23.506 | 1.00 | 0.00 |
| ATOM | 101 | C | THR | 1 | 437 | 24.902 | 49.277 | 22.916 | 1.00 | 0.00 |
| ATOM | 102 | O | THR | 1 | 437 | 24.569 | 50.445 | 23.116 | 1.00 | 0.00 |
| ATOM | 103 | CB | THR | 1 | 437 | 26.061 | 48.651 | 25.022 | 1.00 | 0.00 |
| ATOM | 104 | OG1 | THR | 1 | 437 | 27.343 | 48.873 | 25.650 | 1.00 | 0.00 |
| ATOM | 105 | CG2 | THR | 1 | 437 | 25.354 | 47.371 | 25.472 | 1.00 | 0.00 |
| ATOM | 106 | H | THR | 1 | 437 | 27.906 | 49.970 | 23.724 | 1.00 | 0.00 |
| ATOM | 107 | HG1 | THR | 1 | 437 | 27.458 | 49.821 | 25.588 | 1.00 | 0.00 |
| ATOM | 108 | N | ILE | 1 | 438 | 24.164 | 48.387 | 22.228 | 1.00 | 0.00 |
| ATOM | 109 | CA | ILE | 1 | 438 | 22.799 | 48.710 | 21.782 | 1.00 | 0.00 |
| ATOM | 110 | C | ILE | 1 | 438 | 21.877 | 49.189 | 22.906 | 1.00 | 0.00 |
| ATOM | 111 | O | ILE | 1 | 438 | 21.039 | 50.075 | 22.742 | 1.00 | 0.00 |
| ATOM | 112 | CB | ILE | 1 | 438 | 22.188 | 47.517 | 21.018 | 1.00 | 0.00 |
| ATOM | 113 | CG1 | ILE | 1 | 438 | 20.726 | 47.752 | 20.614 | 1.00 | 0.00 |
| ATOM | 114 | CG2 | ILE | 1 | 438 | 22.299 | 46.215 | 21.825 | 1.00 | 0.00 |
| ATOM | 115 | CD1 | ILE | 1 | 438 | 20.528 | 48.811 | 19.532 | 1.00 | 0.00 |
| ATOM | 116 | H | ILE | 1 | 438 | 24.544 | 47.463 | 22.204 | 1.00 | 0.00 |
| ATOM | 117 | N | LEU | 1 | 439 | 22.123 | 48.579 | 24.080 | 1.00 | 0.00 |
| ATOM | 118 | CA | LEU | 1 | 439 | 21.353 | 49.012 | 25.236 | 1.00 | 0.00 |
| ATOM | 119 | C | LEU | 1 | 439 | 21.746 | 50.402 | 25.702 | 1.00 | 0.00 |
| ATOM | 120 | O | LEU | 1 | 439 | 20.925 | 51.199 | 26.151 | 1.00 | 0.00 |
| ATOM | 121 | CB | LEU | 1 | 439 | 21.499 | 47.982 | 26.361 | 1.00 | 0.00 |
| ATOM | 122 | CG | LEU | 1 | 439 | 20.608 | 48.222 | 27.585 | 1.00 | 0.00 |
| ATOM | 123 | CD1 | LEU | 1 | 439 | 19.117 | 48.142 | 27.249 | 1.00 | 0.00 |
| ATOM | 124 | CD2 | LEU | 1 | 439 | 20.981 | 47.291 | 28.739 | 1.00 | 0.00 |
| ATOM | 125 | H | LEU | 1 | 439 | 22.909 | 47.975 | 24.181 | 1.00 | 0.00 |
| ATOM | 126 | N | GLU | 1 | 440 | 23.049 | 50.678 | 25.615 | 1.00 | 0.00 |
| ATOM | 127 | CA | GLU | 1 | 440 | 23.420 | 51.995 | 26.127 | 1.00 | 0.00 |
| ATOM | 128 | C | GLU | 1 | 440 | 23.181 | 53.116 | 25.136 | 1.00 | 0.00 |
| ATOM | 129 | O | GLU | 1 | 440 | 23.105 | 52.904 | 23.920 | 1.00 | 0.00 |
| ATOM | 130 | CB | GLU | 1 | 440 | 24.872 | 52.018 | 26.609 | 1.00 | 0.00 |
| ATOM | 131 | CG | GLU | 1 | 440 | 25.882 | 52.122 | 25.458 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 132 | CD | GLU | 1 | 440 | 27.302 | 52.026 | 25.950 | 1.00 | 0.00 |
| ATOM | 133 | OE1 | GLU | 1 | 440 | 27.548 | 51.383 | 26.951 | 1.00 | 0.00 |
| ATOM | 134 | OE2 | GLU | 1 | 440 | 28.187 | 52.576 | 25.323 | 1.00 | 0.00 |
| ATOM | 135 | H | GLU | 1 | 440 | 23.690 | 50.027 | 25.219 | 1.00 | 0.00 |
| ATOM | 136 | N | GLU | 1 | 441 | 23.147 | 54.311 | 25.721 | 1.00 | 0.00 |
| ATOM | 137 | CA | GLU | 1 | 441 | 23.125 | 55.552 | 24.951 | 1.00 | 0.00 |
| ATOM | 138 | C | GLU | 1 | 441 | 24.540 | 55.907 | 24.428 | 1.00 | 0.00 |
| ATOM | 139 | O | GLU | 1 | 441 | 25.321 | 54.975 | 24.200 | 1.00 | 0.00 |
| ATOM | 140 | CB | GLU | 1 | 441 | 22.391 | 56.554 | 25.864 | 1.00 | 0.00 |
| ATOM | 141 | CG | GLU | 1 | 441 | 20.977 | 56.094 | 26.255 | 1.00 | 0.00 |
| ATOM | 142 | CD | GLU | 1 | 441 | 20.153 | 55.780 | 25.018 | 1.00 | 0.00 |
| ATOM | 143 | OE1 | GLU | 1 | 441 | 19.756 | 56.694 | 24.311 | 1.00 | 0.00 |
| ATOM | 144 | OE2 | GLU | 1 | 441 | 19.899 | 54.613 | 24.740 | 1.00 | 0.00 |
| ATOM | 145 | H | GLU | 1 | 441 | 23.176 | 54.353 | 26.718 | 1.00 | 0.00 |
| ATOM | 146 | N | PRO | 1 | 442 | 24.892 | 57.209 | 24.202 | 1.00 | 0.00 |
| ATOM | 147 | CA | PRO | 1 | 442 | 24.013 | 58.315 | 23.765 | 1.00 | 0.00 |
| ATOM | 148 | C | PRO | 1 | 442 | 23.258 | 58.135 | 22.446 | 1.00 | 0.00 |
| ATOM | 149 | O | PRO | 1 | 442 | 22.629 | 59.051 | 21.904 | 1.00 | 0.00 |
| ATOM | 150 | CB | PRO | 1 | 442 | 24.957 | 59.521 | 23.748 | 1.00 | 0.00 |
| ATOM | 151 | CG | PRO | 1 | 442 | 26.375 | 58.989 | 23.673 | 1.00 | 0.00 |
| ATOM | 152 | CD | PRO | 1 | 442 | 26.284 | 57.619 | 24.322 | 1.00 | 0.00 |
| ATOM | 153 | N | TYR | 1 | 443 | 23.320 | 56.904 | 21.920 | 1.00 | 0.00 |
| ATOM | 154 | CA | TYR | 1 | 443 | 22.768 | 56.662 | 20.599 | 1.00 | 0.00 |
| ATOM | 155 | C | TYR | 1 | 443 | 21.309 | 56.203 | 20.615 | 1.00 | 0.00 |
| ATOM | 156 | O | TYR | 1 | 443 | 20.947 | 55.060 | 20.353 | 1.00 | 0.00 |
| ATOM | 157 | CB | TYR | 1 | 443 | 23.784 | 55.791 | 19.828 | 1.00 | 0.00 |
| ATOM | 158 | CG | TYR | 1 | 443 | 25.192 | 56.289 | 20.146 | 1.00 | 0.00 |
| ATOM | 159 | CD1 | TYR | 1 | 443 | 25.596 | 57.572 | 19.711 | 1.00 | 0.00 |
| ATOM | 160 | CD2 | TYR | 1 | 443 | 26.050 | 55.482 | 20.928 | 1.00 | 0.00 |
| ATOM | 161 | CE1 | TYR | 1 | 443 | 26.811 | 58.107 | 20.178 | 1.00 | 0.00 |
| ATOM | 162 | CE2 | TYR | 1 | 443 | 27.277 | 56.010 | 21.378 | 1.00 | 0.00 |
| ATOM | 163 | CZ | TYR | 1 | 443 | 27.610 | 57.344 | 21.057 | 1.00 | 0.00 |
| ATOM | 164 | OH | TYR | 1 | 443 | 28.705 | 57.952 | 21.661 | 1.00 | 0.00 |
| ATOM | 165 | H | TYR | 1 | 443 | 23.912 | 56.247 | 22.377 | 1.00 | 0.00 |
| ATOM | 166 | HH | TYR | 1 | 443 | 29.423 | 57.312 | 21.617 | 1.00 | 0.00 |
| ATOM | 167 | N | VAL | 1 | 444 | 20.500 | 57.225 | 20.940 | 1.00 | 0.00 |
| ATOM | 168 | CA | VAL | 1 | 444 | 19.027 | 57.190 | 20.917 | 1.00 | 0.00 |
| ATOM | 169 | C | VAL | 1 | 444 | 18.253 | 55.867 | 21.029 | 1.00 | 0.00 |
| ATOM | 170 | O | VAL | 1 | 444 | 17.637 | 55.359 | 20.079 | 1.00 | 0.00 |
| ATOM | 171 | CB | VAL | 1 | 444 | 18.488 | 58.050 | 19.754 | 1.00 | 0.00 |
| ATOM | 172 | CG1 | VAL | 1 | 444 | 17.028 | 58.457 | 19.988 | 1.00 | 0.00 |
| ATOM | 173 | CG2 | VAL | 1 | 444 | 19.350 | 59.294 | 19.511 | 1.00 | 0.00 |
| ATOM | 174 | H | VAL | 1 | 444 | 20.984 | 58.057 | 21.205 | 1.00 | 0.00 |
| ATOM | 175 | N | LEU | 1 | 445 | 18.238 | 55.392 | 22.276 | 1.00 | 0.00 |
| ATOM | 176 | CA | LEU | 1 | 445 | 17.191 | 54.528 | 22.805 | 1.00 | 0.00 |
| ATOM | 177 | C | LEU | 1 | 445 | 17.003 | 53.178 | 22.162 | 1.00 | 0.00 |
| ATOM | 178 | O | LEU | 1 | 445 | 16.267 | 52.982 | 21.190 | 1.00 | 0.00 |
| ATOM | 179 | CB | LEU | 1 | 445 | 15.861 | 55.278 | 22.942 | 1.00 | 0.00 |
| ATOM | 180 | CG | LEU | 1 | 445 | 15.926 | 56.363 | 24.020 | 1.00 | 0.00 |
| ATOM | 181 | CD1 | LEU | 1 | 445 | 14.686 | 57.257 | 24.009 | 1.00 | 0.00 |
| ATOM | 182 | CD2 | LEU | 1 | 445 | 16.190 | 55.768 | 25.405 | 1.00 | 0.00 |
| ATOM | 183 | H | LEU | 1 | 445 | 19.012 | 55.682 | 22.834 | 1.00 | 0.00 |
| ATOM | 184 | N | PHE | 1 | 446 | 17.667 | 52.243 | 22.863 | 1.00 | 0.00 |
| ATOM | 185 | CA | PHE | 1 | 446 | 17.499 | 50.792 | 22.711 | 1.00 | 0.00 |
| ATOM | 186 | C | PHE | 1 | 446 | 16.341 | 50.249 | 21.880 | 1.00 | 0.00 |
| ATOM | 187 | O | PHE | 1 | 446 | 15.163 | 50.174 | 22.243 | 1.00 | 0.00 |
| ATOM | 188 | CB | PHE | 1 | 446 | 17.601 | 50.086 | 24.075 | 1.00 | 0.00 |
| ATOM | 189 | CG | PHE | 1 | 446 | 16.942 | 50.872 | 25.190 | 1.00 | 0.00 |
| ATOM | 190 | CD1 | PHE | 1 | 446 | 17.754 | 51.626 | 26.066 | 1.00 | 0.00 |
| ATOM | 191 | CD2 | PHE | 1 | 446 | 15.539 | 50.838 | 25.347 | 1.00 | 0.00 |
| ATOM | 192 | CE1 | PHE | 1 | 446 | 17.159 | 52.353 | 27.115 | 1.00 | 0.00 |
| ATOM | 193 | CE2 | PHE | 1 | 446 | 14.941 | 51.565 | 26.395 | 1.00 | 0.00 |
| ATOM | 194 | CZ | PHE | 1 | 446 | 15.758 | 52.314 | 27.269 | 1.00 | 0.00 |
| ATOM | 195 | H | PHE | 1 | 446 | 18.393 | 52.615 | 23.444 | 1.00 | 0.00 |
| ATOM | 196 | N | LYS | 1 | 447 | 16.779 | 49.840 | 20.674 | 1.00 | 0.00 |
| ATOM | 197 | CA | LYS | 1 | 447 | 15.885 | 49.287 | 19.657 | 1.00 | 0.00 |
| ATOM | 198 | C | LYS | 1 | 447 | 16.685 | 48.583 | 18.569 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 199 | O | LYS | 1 | 447 | 17.061 | 49.213 | 17.589 | 1.00 | 0.00 |
| ATOM | 200 | CB | LYS | 1 | 447 | 15.052 | 50.424 | 19.041 | 1.00 | 0.00 |
| ATOM | 201 | CG | LYS | 1 | 447 | 13.626 | 50.082 | 18.589 | 1.00 | 0.00 |
| ATOM | 202 | CD | LYS | 1 | 447 | 13.453 | 49.205 | 17.341 | 1.00 | 0.00 |
| ATOM | 203 | CE | LYS | 1 | 447 | 13.982 | 49.807 | 16.031 | 1.00 | 0.00 |
| ATOM | 204 | NZ | LYS | 1 | 447 | 15.345 | 49.332 | 15.781 | 1.00 | 0.00 |
| ATOM | 205 | H | LYS | 1 | 447 | 17.753 | 49.971 | 20.474 | 1.00 | 0.00 |
| ATOM | 206 | 1HZ | LYS | 1 | 447 | 15.427 | 48.333 | 16.052 | 1.00 | 0.00 |
| ATOM | 207 | 2HZ | LYS | 1 | 447 | 15.621 | 49.376 | 14.781 | 1.00 | 0.00 |
| ATOM | 208 | 3HZ | LYS | 1 | 447 | 16.055 | 49.850 | 16.335 | 1.00 | 0.00 |
| ATOM | 209 | N | LYS | 1 | 448 | 16.922 | 47.273 | 18.750 | 1.00 | 0.00 |
| ATOM | 210 | CA | LYS | 1 | 448 | 17.628 | 46.529 | 17.696 | 1.00 | 0.00 |
| ATOM | 211 | C | LYS | 1 | 448 | 16.842 | 46.428 | 16.389 | 1.00 | 0.00 |
| ATOM | 212 | O | LYS | 1 | 448 | 15.635 | 46.656 | 16.339 | 1.00 | 0.00 |
| ATOM | 213 | CB | LYS | 1 | 448 | 18.000 | 45.121 | 18.199 | 1.00 | 0.00 |
| ATOM | 214 | CG | LYS | 1 | 448 | 19.423 | 44.956 | 18.762 | 1.00 | 0.00 |
| ATOM | 215 | CD | LYS | 1 | 448 | 20.490 | 44.980 | 17.663 | 1.00 | 0.00 |
| ATOM | 216 | CE | LYS | 1 | 448 | 21.961 | 45.141 | 18.082 | 1.00 | 0.00 |
| ATOM | 217 | NZ | LYS | 1 | 448 | 22.795 | 45.329 | 16.885 | 1.00 | 0.00 |
| ATOM | 218 | H | LYS | 1 | 448 | 16.473 | 46.795 | 19.504 | 1.00 | 0.00 |
| ATOM | 219 | 1HZ | LYS | 1 | 448 | 22.871 | 44.446 | 16.342 | 1.00 | 0.00 |
| ATOM | 220 | 2HZ | LYS | 1 | 448 | 22.369 | 46.042 | 16.256 | 1.00 | 0.00 |
| ATOM | 221 | 3HZ | LYS | 1 | 448 | 23.770 | 45.603 | 17.121 | 1.00 | 0.00 |
| ATOM | 222 | N | SER | 1 | 449 | 17.589 | 46.066 | 15.342 | 1.00 | 0.00 |
| ATOM | 223 | CA | SER | 1 | 449 | 16.982 | 45.670 | 14.065 | 1.00 | 0.00 |
| ATOM | 224 | C | SER | 1 | 449 | 17.880 | 44.735 | 13.261 | 1.00 | 0.00 |
| ATOM | 225 | O | SER | 1 | 449 | 17.806 | 44.644 | 12.036 | 1.00 | 0.00 |
| ATOM | 226 | CB | SER | 1 | 449 | 16.613 | 46.882 | 13.186 | 1.00 | 0.00 |
| ATOM | 227 | OG | SER | 1 | 449 | 16.525 | 48.091 | 13.970 | 1.00 | 0.00 |
| ATOM | 228 | H | SER | 1 | 449 | 18.578 | 46.234 | 15.380 | 1.00 | 0.00 |
| ATOM | 229 | HG | SER | 1 | 449 | 17.450 | 48.259 | 14.182 | 1.00 | 0.00 |
| ATOM | 230 | N | ASP | 1 | 450 | 18.768 | 44.051 | 14.008 | 1.00 | 0.00 |
| ATOM | 231 | CA | ASP | 1 | 450 | 19.902 | 43.386 | 13.364 | 1.00 | 0.00 |
| ATOM | 232 | C | ASP | 1 | 450 | 19.627 | 42.151 | 12.518 | 1.00 | 0.00 |
| ATOM | 233 | O | ASP | 1 | 450 | 19.835 | 41.013 | 12.911 | 1.00 | 0.00 |
| ATOM | 234 | CB | ASP | 1 | 450 | 21.009 | 43.091 | 14.383 | 1.00 | 0.00 |
| ATOM | 235 | CG | ASP | 1 | 450 | 22.343 | 43.743 | 14.030 | 1.00 | 0.00 |
| ATOM | 236 | OD1 | ASP | 1 | 450 | 23.246 | 43.666 | 14.855 | 1.00 | 0.00 |
| ATOM | 237 | OD2 | ASP | 1 | 450 | 22.496 | 44.333 | 12.961 | 1.00 | 0.00 |
| ATOM | 238 | H | ASP | 1 | 450 | 18.693 | 44.094 | 14.999 | 1.00 | 0.00 |
| ATOM | 239 | N | LYS | 1 | 451 | 19.209 | 42.448 | 11.285 | 1.00 | 0.00 |
| ATOM | 240 | CA | LYS | 1 | 451 | 19.489 | 41.590 | 10.132 | 1.00 | 0.00 |
| ATOM | 241 | C | LYS | 1 | 451 | 20.968 | 41.225 | 10.095 | 1.00 | 0.00 |
| ATOM | 242 | O | LYS | 1 | 451 | 21.794 | 42.104 | 10.338 | 1.00 | 0.00 |
| ATOM | 243 | CB | LYS | 1 | 451 | 19.069 | 42.321 | 8.835 | 1.00 | 0.00 |
| ATOM | 244 | CG | LYS | 1 | 451 | 19.845 | 43.600 | 8.444 | 1.00 | 0.00 |
| ATOM | 245 | CD | LYS | 1 | 451 | 19.617 | 44.819 | 9.350 | 1.00 | 0.00 |
| ATOM | 246 | CE | LYS | 1 | 451 | 20.881 | 45.542 | 9.835 | 1.00 | 0.00 |
| ATOM | 247 | NZ | LYS | 1 | 451 | 21.822 | 44.664 | 10.551 | 1.00 | 0.00 |
| ATOM | 248 | H | LYS | 1 | 451 | 18.751 | 43.322 | 11.155 | 1.00 | 0.00 |
| ATOM | 249 | 1HZ | LYS | 1 | 451 | 22.220 | 43.888 | 9.980 | 1.00 | 0.00 |
| ATOM | 250 | 2HZ | LYS | 1 | 451 | 22.639 | 45.223 | 10.859 | 1.00 | 0.00 |
| ATOM | 251 | 3HZ | LYS | 1 | 451 | 21.482 | 44.255 | 11.443 | 1.00 | 0.00 |
| ATOM | 252 | N | PRO | 1 | 452 | 21.274 | 39.939 | 9.810 | 1.00 | 0.00 |
| ATOM | 253 | CA | PRO | 1 | 452 | 22.657 | 39.447 | 9.917 | 1.00 | 0.00 |
| ATOM | 254 | C | PRO | 1 | 452 | 23.690 | 40.087 | 8.993 | 1.00 | 0.00 |
| ATOM | 255 | O | PRO | 1 | 452 | 24.892 | 39.921 | 9.170 | 1.00 | 0.00 |
| ATOM | 256 | CB | PRO | 1 | 452 | 22.496 | 37.936 | 9.708 | 1.00 | 0.00 |
| ATOM | 257 | CG | PRO | 1 | 452 | 21.211 | 37.774 | 8.900 | 1.00 | 0.00 |
| ATOM | 258 | CD | PRO | 1 | 452 | 20.332 | 38.887 | 9.454 | 1.00 | 0.00 |
| ATOM | 259 | N | LEU | 1 | 453 | 23.191 | 40.842 | 8.000 | 1.00 | 0.00 |
| ATOM | 260 | CA | LEU | 1 | 453 | 24.118 | 41.808 | 7.421 | 1.00 | 0.00 |
| ATOM | 261 | C | LEU | 1 | 453 | 24.117 | 43.067 | 8.268 | 1.00 | 0.00 |
| ATOM | 262 | O | LEU | 1 | 453 | 23.063 | 43.664 | 8.484 | 1.00 | 0.00 |
| ATOM | 263 | CB | LEU | 1 | 453 | 23.724 | 42.119 | 5.974 | 1.00 | 0.00 |
| ATOM | 264 | CG | LEU | 1 | 453 | 24.708 | 43.039 | 5.241 | 1.00 | 0.00 |
| ATOM | 265 | CD1 | LEU | 1 | 453 | 26.102 | 42.419 | 5.121 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 266 | CD2 | LEU | 1 | 453 | 24.160 | 43.485 | 3.886 | 1.00 | 0.00 |
| ATOM | 267 | H | LEU | 1 | 453 | 22.211 | 40.846 | 7.808 | 1.00 | 0.00 |
| ATOM | 268 | N | TYR | 1 | 454 | 25.329 | 43.427 | 8.730 | 1.00 | 0.00 |
| ATOM | 269 | CA | TYR | 1 | 454 | 25.478 | 44.528 | 9.695 | 1.00 | 0.00 |
| ATOM | 270 | C | TYR | 1 | 454 | 24.631 | 45.786 | 9.487 | 1.00 | 0.00 |
| ATOM | 271 | O | TYR | 1 | 454 | 23.898 | 46.188 | 10.391 | 1.00 | 0.00 |
| ATOM | 272 | CB | TYR | 1 | 454 | 26.962 | 44.829 | 9.991 | 1.00 | 0.00 |
| ATOM | 273 | CG | TYR | 1 | 454 | 27.729 | 45.364 | 8.800 | 1.00 | 0.00 |
| ATOM | 274 | CD1 | TYR | 1 | 454 | 28.152 | 44.479 | 7.785 | 1.00 | 0.00 |
| ATOM | 275 | CD2 | TYR | 1 | 454 | 28.016 | 46.743 | 8.748 | 1.00 | 0.00 |
| ATOM | 276 | CE1 | TYR | 1 | 454 | 28.868 | 44.985 | 6.688 | 1.00 | 0.00 |
| ATOM | 277 | CE2 | TYR | 1 | 454 | 28.735 | 47.250 | 7.654 | 1.00 | 0.00 |
| ATOM | 278 | CZ | TYR | 1 | 454 | 29.146 | 46.366 | 6.636 | 1.00 | 0.00 |
| ATOM | 279 | OH | TYR | 1 | 454 | 29.831 | 46.879 | 5.548 | 1.00 | 0.00 |
| ATOM | 280 | H | TYR | 1 | 454 | 26.065 | 42.779 | 8.535 | 1.00 | 0.00 |
| ATOM | 281 | HH | TYR | 1 | 454 | 30.640 | 47.262 | 5.894 | 1.00 | 0.00 |
| ATOM | 282 | N | GLY | 1 | 455 | 24.681 | 46.322 | 8.248 | 1.00 | 0.00 |
| ATOM | 283 | CA | GLY | 1 | 455 | 23.647 | 47.259 | 7.782 | 1.00 | 0.00 |
| ATOM | 284 | C | GLY | 1 | 455 | 23.288 | 48.432 | 8.689 | 1.00 | 0.00 |
| ATOM | 285 | O | GLY | 1 | 455 | 24.019 | 48.788 | 9.613 | 1.00 | 0.00 |
| ATOM | 286 | H | GLY | 1 | 455 | 25.419 | 46.012 | 7.648 | 1.00 | 0.00 |
| ATOM | 287 | N | ASN | 1 | 456 | 22.123 | 49.025 | 8.387 | 1.00 | 0.00 |
| ATOM | 288 | CA | ASN | 1 | 456 | 21.833 | 50.251 | 9.139 | 1.00 | 0.00 |
| ATOM | 289 | C | ASN | 1 | 456 | 21.053 | 50.088 | 10.423 | 1.00 | 0.00 |
| ATOM | 290 | O | ASN | 1 | 456 | 20.036 | 50.736 | 10.675 | 1.00 | 0.00 |
| ATOM | 291 | CB | ASN | 1 | 456 | 21.223 | 51.325 | 8.236 | 1.00 | 0.00 |
| ATOM | 292 | CG | ASN | 1 | 456 | 22.366 | 52.002 | 7.514 | 1.00 | 0.00 |
| ATOM | 293 | OD1 | ASN | 1 | 456 | 23.364 | 51.381 | 7.172 | 1.00 | 0.00 |
| ATOM | 294 | ND2 | ASN | 1 | 456 | 22.227 | 53.321 | 7.365 | 1.00 | 0.00 |
| ATOM | 295 | H | ASN | 1 | 456 | 21.593 | 48.740 | 7.592 | 1.00 | 0.00 |
| ATOM | 296 | 1HD2 | ASN | 1 | 456 | 23.042 | 53.793 | 7.015 | 1.00 | 0.00 |
| ATOM | 297 | 2HD2 | ASN | 1 | 456 | 21.416 | 53.865 | 7.573 | 1.00 | 0.00 |
| ATOM | 298 | N | ASP | 1 | 457 | 21.581 | 49.161 | 11.228 | 1.00 | 0.00 |
| ATOM | 299 | CA | ASP | 1 | 457 | 21.077 | 49.019 | 12.587 | 1.00 | 0.00 |
| ATOM | 300 | C | ASP | 1 | 457 | 21.906 | 49.828 | 13.563 | 1.00 | 0.00 |
| ATOM | 301 | O | ASP | 1 | 457 | 23.113 | 50.011 | 13.396 | 1.00 | 0.00 |
| ATOM | 302 | CB | ASP | 1 | 457 | 21.032 | 47.544 | 13.006 | 1.00 | 0.00 |
| ATOM | 303 | CG | ASP | 1 | 457 | 20.298 | 47.378 | 14.326 | 1.00 | 0.00 |
| ATOM | 304 | OD1 | ASP | 1 | 457 | 20.704 | 46.551 | 15.134 | 1.00 | 0.00 |
| ATOM | 305 | OD2 | ASP | 1 | 457 | 19.316 | 48.080 | 14.557 | 1.00 | 0.00 |
| ATOM | 306 | H | ASP | 1 | 457 | 22.468 | 48.789 | 10.968 | 1.00 | 0.00 |
| ATOM | 307 | N | ARG | 1 | 458 | 21.185 | 50.326 | 14.575 | 1.00 | 0.00 |
| ATOM | 308 | CA | ARG | 1 | 458 | 21.756 | 51.237 | 15.560 | 1.00 | 0.00 |
| ATOM | 309 | C | ARG | 1 | 458 | 22.887 | 50.633 | 16.369 | 1.00 | 0.00 |
| ATOM | 310 | O | ARG | 1 | 458 | 22.698 | 49.911 | 17.342 | 1.00 | 0.00 |
| ATOM | 311 | CB | ARG | 1 | 458 | 20.621 | 51.755 | 16.451 | 1.00 | 0.00 |
| ATOM | 312 | CG | ARG | 1 | 458 | 20.970 | 52.868 | 17.446 | 1.00 | 0.00 |
| ATOM | 313 | CD | ARG | 1 | 458 | 20.934 | 52.394 | 18.902 | 1.00 | 0.00 |
| ATOM | 314 | NE | ARG | 1 | 458 | 22.274 | 52.174 | 19.447 | 1.00 | 0.00 |
| ATOM | 315 | CZ | ARG | 1 | 458 | 22.528 | 52.312 | 20.772 | 1.00 | 0.00 |
| ATOM | 316 | NH1 | ARG | 1 | 458 | 23.775 | 52.156 | 21.205 | 1.00 | 0.00 |
| ATOM | 317 | NH2 | ARG | 1 | 458 | 21.545 | 52.578 | 21.631 | 1.00 | 0.00 |
| ATOM | 318 | H | ARG | 1 | 458 | 20.291 | 49.908 | 14.714 | 1.00 | 0.00 |
| ATOM | 319 | HE | ARG | 1 | 458 | 23.025 | 51.873 | 18.851 | 1.00 | 0.00 |
| ATOM | 320 | 1HH1 | ARG | 1 | 458 | 24.539 | 52.170 | 20.548 | 1.00 | 0.00 |
| ATOM | 321 | 2HH1 | ARG | 1 | 458 | 23.971 | 52.020 | 22.183 | 1.00 | 0.00 |
| ATOM | 322 | 1HH2 | ARG | 1 | 458 | 21.733 | 52.667 | 22.616 | 1.00 | 0.00 |
| ATOM | 323 | 2HH2 | ARG | 1 | 458 | 20.600 | 52.655 | 21.308 | 1.00 | 0.00 |
| ATOM | 324 | N | PHE | 1 | 459 | 24.093 | 50.987 | 15.937 | 1.00 | 0.00 |
| ATOM | 325 | CA | PHE | 1 | 459 | 25.211 | 50.757 | 16.842 | 1.00 | 0.00 |
| ATOM | 326 | C | PHE | 1 | 459 | 25.494 | 52.044 | 17.589 | 1.00 | 0.00 |
| ATOM | 327 | O | PHE | 1 | 459 | 25.107 | 52.202 | 18.751 | 1.00 | 0.00 |
| ATOM | 328 | CB | PHE | 1 | 459 | 26.424 | 50.202 | 16.081 | 1.00 | 0.00 |
| ATOM | 329 | CG | PHE | 1 | 459 | 26.018 | 48.996 | 15.259 | 1.00 | 0.00 |
| ATOM | 330 | CD1 | PHE | 1 | 459 | 26.017 | 49.096 | 13.850 | 1.00 | 0.00 |
| ATOM | 331 | CD2 | PHE | 1 | 459 | 25.641 | 47.796 | 15.903 | 1.00 | 0.00 |
| ATOM | 332 | CE1 | PHE | 1 | 459 | 25.624 | 47.988 | 13.074 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 333 | CE2 | PHE | 1 | 459 | 25.249 | 46.687 | 15.129 | 1.00 | 0.00 |
| ATOM | 334 | CZ | PHE | 1 | 459 | 25.240 | 46.795 | 13.723 | 1.00 | 0.00 |
| ATOM | 335 | H | PHE | 1 | 459 | 24.157 | 51.522 | 15.097 | 1.00 | 0.00 |
| ATOM | 336 | N | GLU | 1 | 460 | 26.069 | 52.992 | 16.816 | 1.00 | 0.00 |
| ATOM | 337 | CA | GLU | 1 | 460 | 26.318 | 54.335 | 17.332 | 1.00 | 0.00 |
| ATOM | 338 | C | GLU | 1 | 460 | 26.015 | 55.451 | 16.314 | 1.00 | 0.00 |
| ATOM | 339 | O | GLU | 1 | 460 | 25.295 | 55.185 | 15.352 | 1.00 | 0.00 |
| ATOM | 340 | CB | GLU | 1 | 460 | 27.650 | 54.371 | 18.109 | 1.00 | 0.00 |
| ATOM | 341 | CG | GLU | 1 | 460 | 28.991 | 54.650 | 17.432 | 1.00 | 0.00 |
| ATOM | 342 | CD | GLU | 1 | 460 | 29.593 | 55.840 | 18.158 | 1.00 | 0.00 |
| ATOM | 343 | OE1 | GLU | 1 | 460 | 28.923 | 56.850 | 18.264 | 1.00 | 0.00 |
| ATOM | 344 | OE2 | GLU | 1 | 460 | 30.723 | 55.793 | 18.622 | 1.00 | 0.00 |
| ATOM | 345 | H | GLU | 1 | 460 | 26.290 | 52.811 | 15.859 | 1.00 | 0.00 |
| ATOM | 346 | N | GLY | 1 | 461 | 26.466 | 56.695 | 16.584 | 1.00 | 0.00 |
| ATOM | 347 | CA | GLY | 1 | 461 | 25.962 | 57.844 | 15.814 | 1.00 | 0.00 |
| ATOM | 348 | C | GLY | 1 | 461 | 27.014 | 58.898 | 15.473 | 1.00 | 0.00 |
| ATOM | 349 | O | GLY | 1 | 461 | 27.321 | 59.189 | 14.312 | 1.00 | 0.00 |
| ATOM | 350 | H | GLY | 1 | 461 | 27.152 | 56.871 | 17.292 | 1.00 | 0.00 |
| ATOM | 351 | N | TYR | 1 | 462 | 27.595 | 59.435 | 16.570 | 1.00 | 0.00 |
| ATOM | 352 | CA | TYR | 1 | 462 | 28.710 | 60.373 | 16.414 | 1.00 | 0.00 |
| ATOM | 353 | C | TYR | 1 | 462 | 29.918 | 59.729 | 15.764 | 1.00 | 0.00 |
| ATOM | 354 | O | TYR | 1 | 462 | 30.716 | 60.354 | 15.063 | 1.00 | 0.00 |
| ATOM | 355 | CB | TYR | 1 | 462 | 29.074 | 60.997 | 17.771 | 1.00 | 0.00 |
| ATOM | 356 | CG | TYR | 1 | 462 | 30.079 | 62.123 | 17.618 | 1.00 | 0.00 |
| ATOM | 357 | CD1 | TYR | 1 | 462 | 31.386 | 61.950 | 18.122 | 1.00 | 0.00 |
| ATOM | 358 | CD2 | TYR | 1 | 462 | 29.685 | 63.316 | 16.978 | 1.00 | 0.00 |
| ATOM | 359 | CE1 | TYR | 1 | 462 | 32.317 | 62.996 | 17.985 | 1.00 | 0.00 |
| ATOM | 360 | CE2 | TYR | 1 | 462 | 30.614 | 64.358 | 16.841 | 1.00 | 0.00 |
| ATOM | 361 | CZ | TYR | 1 | 462 | 31.918 | 64.188 | 17.346 | 1.00 | 0.00 |
| ATOM | 362 | OH | TYR | 1 | 462 | 32.832 | 65.223 | 17.202 | 1.00 | 0.00 |
| ATOM | 363 | H | TYR | 1 | 462 | 27.418 | 58.980 | 17.440 | 1.00 | 0.00 |
| ATOM | 364 | HH | TYR | 1 | 462 | 32.507 | 65.837 | 16.547 | 1.00 | 0.00 |
| ATOM | 365 | N | CYS | 1 | 463 | 29.986 | 58.413 | 16.006 | 1.00 | 0.00 |
| ATOM | 366 | CA | CYS | 1 | 463 | 30.912 | 57.668 | 15.179 | 1.00 | 0.00 |
| ATOM | 367 | C | CYS | 1 | 463 | 30.295 | 56.846 | 14.073 | 1.00 | 0.00 |
| ATOM | 368 | O | CYS | 1 | 463 | 30.993 | 56.278 | 13.244 | 1.00 | 0.00 |
| ATOM | 369 | CB | CYS | 1 | 463 | 31.914 | 56.882 | 16.009 | 1.00 | 0.00 |
| ATOM | 370 | SG | CYS | 1 | 463 | 32.876 | 57.991 | 17.077 | 1.00 | 0.00 |
| ATOM | 371 | H | CYS | 1 | 463 | 29.406 | 57.960 | 16.679 | 1.00 | 0.00 |
| ATOM | 372 | N | LEU | 1 | 464 | 28.959 | 56.857 | 13.992 | 1.00 | 0.00 |
| ATOM | 373 | CA | LEU | 1 | 464 | 28.435 | 56.438 | 12.685 | 1.00 | 0.00 |
| ATOM | 374 | C | LEU | 1 | 464 | 28.868 | 57.374 | 11.562 | 1.00 | 0.00 |
| ATOM | 375 | O | LEU | 1 | 464 | 29.049 | 56.991 | 10.410 | 1.00 | 0.00 |
| ATOM | 376 | CB | LEU | 1 | 464 | 26.913 | 56.272 | 12.718 | 1.00 | 0.00 |
| ATOM | 377 | CG | LEU | 1 | 464 | 26.271 | 55.636 | 11.480 | 1.00 | 0.00 |
| ATOM | 378 | CD1 | LEU | 1 | 464 | 26.795 | 54.226 | 11.200 | 1.00 | 0.00 |
| ATOM | 379 | CD2 | LEU | 1 | 464 | 24.745 | 55.660 | 11.577 | 1.00 | 0.00 |
| ATOM | 380 | H | LEU | 1 | 464 | 28.395 | 57.273 | 14.702 | 1.00 | 0.00 |
| ATOM | 381 | N | ASP | 1 | 465 | 29.063 | 58.647 | 11.954 | 1.00 | 0.00 |
| ATOM | 382 | CA | ASP | 1 | 465 | 29.816 | 59.482 | 11.028 | 1.00 | 0.00 |
| ATOM | 383 | C | ASP | 1 | 465 | 31.322 | 59.508 | 11.249 | 1.00 | 0.00 |
| ATOM | 384 | O | ASP | 1 | 465 | 32.080 | 59.566 | 10.286 | 1.00 | 0.00 |
| ATOM | 385 | CB | ASP | 1 | 465 | 29.218 | 60.891 | 10.934 | 1.00 | 0.00 |
| ATOM | 386 | CG | ASP | 1 | 465 | 29.255 | 61.615 | 12.264 | 1.00 | 0.00 |
| ATOM | 387 | OD1 | ASP | 1 | 465 | 28.242 | 61.640 | 12.958 | 1.00 | 0.00 |
| ATOM | 388 | OD2 | ASP | 1 | 465 | 30.285 | 63.192 | 12.603 | 1.00 | 0.00 |
| ATOM | 389 | H | ASP | 1 | 465 | 28.793 | 59.017 | 12.849 | 1.00 | 0.00 |
| ATOM | 390 | N | LEU | 1 | 466 | 31.739 | 59.472 | 12.531 | 1.00 | 0.00 |
| ATOM | 391 | CA | LEU | 1 | 466 | 33.189 | 59.459 | 12.730 | 1.00 | 0.00 |
| ATOM | 392 | C | LEU | 1 | 466 | 33.908 | 58.221 | 12.225 | 1.00 | 0.00 |
| ATOM | 393 | O | LEU | 1 | 466 | 34.692 | 58.317 | 11.292 | 1.00 | 0.00 |
| ATOM | 394 | CB | LEU | 1 | 466 | 33.591 | 59.787 | 14.168 | 1.00 | 0.00 |
| ATOM | 395 | CG | LEU | 1 | 466 | 34.824 | 60.681 | 14.283 | 1.00 | 0.00 |
| ATOM | 396 | CD1 | LEU | 1 | 466 | 34.586 | 62.050 | 13.643 | 1.00 | 0.00 |
| ATOM | 397 | CD2 | LEU | 1 | 466 | 35.291 | 60.805 | 15.734 | 1.00 | 0.00 |
| ATOM | 398 | H | LEU | 1 | 466 | 31.061 | 59.691 | 13.236 | 1.00 | 0.00 |
| ATOM | 399 | N | LEU | 1 | 467 | 33.628 | 57.059 | 12.836 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 400 | CA | LEU | 1 | 467 | 34.318 | 55.802 | 12.516 | 1.00 | 0.00 |
| ATOM | 401 | C | LEU | 1 | 467 | 34.431 | 55.466 | 11.033 | 1.00 | 0.00 |
| ATOM | 402 | O | LEU | 1 | 467 | 35.434 | 54.937 | 10.544 | 1.00 | 0.00 |
| ATOM | 403 | CB | LEU | 1 | 467 | 33.647 | 54.684 | 13.330 | 1.00 | 0.00 |
| ATOM | 404 | CG | LEU | 1 | 467 | 34.067 | 53.242 | 13.059 | 1.00 | 0.00 |
| ATOM | 405 | CD1 | LEU | 1 | 467 | 34.199 | 52.443 | 14.351 | 1.00 | 0.00 |
| ATOM | 406 | CD2 | LEU | 1 | 467 | 33.148 | 52.552 | 12.049 | 1.00 | 0.00 |
| ATOM | 407 | H | LEU | 1 | 467 | 32.874 | 57.017 | 13.487 | 1.00 | 0.00 |
| ATOM | 408 | N | ARG | 1 | 468 | 33.344 | 55.825 | 10.325 | 1.00 | 0.00 |
| ATOM | 409 | CA | ARG | 1 | 468 | 33.392 | 55.682 | 8.871 | 1.00 | 0.00 |
| ATOM | 410 | C | ARG | 1 | 468 | 34.526 | 56.471 | 8.234 | 1.00 | 0.00 |
| ATOM | 411 | O | ARG | 1 | 468 | 35.390 | 55.933 | 7.543 | 1.00 | 0.00 |
| ATOM | 412 | CB | ARG | 1 | 468 | 32.051 | 56.054 | 8.247 | 1.00 | 0.00 |
| ATOM | 413 | CG | ARG | 1 | 468 | 31.581 | 55.039 | 7.200 | 1.00 | 0.00 |
| ATOM | 414 | CD | ARG | 1 | 468 | 30.537 | 55.596 | 6.221 | 1.00 | 0.00 |
| ATOM | 415 | NE | ARG | 1 | 468 | 31.178 | 56.359 | 5.145 | 1.00 | 0.00 |
| ATOM | 416 | CZ | ARG | 1 | 468 | 31.359 | 57.696 | 5.241 | 1.00 | 0.00 |
| ATOM | 417 | NH1 | ARG | 1 | 468 | 32.095 | 58.314 | 4.327 | 1.00 | 0.00 |
| ATOM | 418 | NH2 | ARG | 1 | 468 | 30.836 | 58.394 | 6.250 | 1.00 | 0.00 |
| ATOM | 419 | H | ARG | 1 | 468 | 32.632 | 56.345 | 10.797 | 1.00 | 0.00 |
| ATOM | 420 | HE | ARG | 1 | 468 | 31.657 | 55.812 | 4.448 | 1.00 | 0.00 |
| ATOM | 421 | 1HH1 | ARG | 1 | 468 | 32.383 | 59.268 | 4.504 | 1.00 | 0.00 |
| ATOM | 422 | 2HH1 | ARG | 1 | 468 | 32.454 | 57.882 | 3.501 | 1.00 | 0.00 |
| ATOM | 423 | 1HH2 | ARG | 1 | 468 | 30.977 | 59.394 | 6.267 | 1.00 | 0.00 |
| ATOM | 424 | 2HH2 | ARG | 1 | 468 | 30.348 | 57.961 | 7.013 | 1.00 | 0.00 |
| ATOM | 425 | N | GLU | 1 | 469 | 34.555 | 57.766 | 8.560 | 1.00 | 0.00 |
| ATOM | 426 | CA | GLU | 1 | 469 | 35.677 | 58.544 | 8.052 | 1.00 | 0.00 |
| ATOM | 427 | C | GLU | 1 | 469 | 37.029 | 58.208 | 8.690 | 1.00 | 0.00 |
| ATOM | 428 | O | GLU | 1 | 469 | 38.083 | 58.416 | 8.105 | 1.00 | 0.00 |
| ATOM | 429 | CB | GLU | 1 | 469 | 35.366 | 60.049 | 8.063 | 1.00 | 0.00 |
| ATOM | 430 | CG | GLU | 1 | 469 | 33.927 | 60.477 | 7.689 | 1.00 | 0.00 |
| ATOM | 431 | CD | GLU | 1 | 469 | 33.465 | 60.204 | 6.254 | 1.00 | 0.00 |
| ATOM | 432 | OE1 | GLU | 1 | 469 | 34.169 | 59.617 | 5.449 | 1.00 | 0.00 |
| ATOM | 433 | OE2 | GLU | 1 | 469 | 32.344 | 60.562 | 5.910 | 1.00 | 0.00 |
| ATOM | 434 | H | GLU | 1 | 469 | 33.874 | 58.176 | 9.168 | 1.00 | 0.00 |
| ATOM | 435 | N | LEU | 1 | 470 | 36.994 | 57.600 | 9.889 | 1.00 | 0.00 |
| ATOM | 436 | CA | LEU | 1 | 470 | 38.250 | 57.067 | 10.436 | 1.00 | 0.00 |
| ATOM | 437 | C | LEU | 1 | 470 | 38.776 | 55.846 | 9.692 | 1.00 | 0.00 |
| ATOM | 438 | O | LEU | 1 | 470 | 39.864 | 55.312 | 9.909 | 1.00 | 0.00 |
| ATOM | 439 | CB | LEU | 1 | 470 | 38.092 | 56.763 | 11.924 | 1.00 | 0.00 |
| ATOM | 440 | CG | LEU | 1 | 470 | 37.965 | 58.019 | 12.782 | 1.00 | 0.00 |
| ATOM | 441 | CD1 | LEU | 1 | 470 | 37.542 | 57.695 | 14.212 | 1.00 | 0.00 |
| ATOM | 442 | CD2 | LEU | 1 | 470 | 39.254 | 58.833 | 12.762 | 1.00 | 0.00 |
| ATOM | 443 | H | LEU | 1 | 470 | 36.101 | 57.426 | 10.308 | 1.00 | 0.00 |
| ATOM | 444 | N | SER | 1 | 471 | 37.937 | 55.386 | 8.764 | 1.00 | 0.00 |
| ATOM | 445 | CA | SER | 1 | 471 | 38.437 | 54.432 | 7.793 | 1.00 | 0.00 |
| ATOM | 446 | C | SER | 1 | 471 | 38.981 | 55.060 | 6.517 | 1.00 | 0.00 |
| ATOM | 447 | O | SER | 1 | 471 | 39.891 | 54.526 | 5.898 | 1.00 | 0.00 |
| ATOM | 448 | CB | SER | 1 | 471 | 37.343 | 53.416 | 7.504 | 1.00 | 0.00 |
| ATOM | 449 | OG | SER | 1 | 471 | 37.138 | 52.609 | 8.665 | 1.00 | 0.00 |
| ATOM | 450 | H | SER | 1 | 471 | 37.018 | 55.774 | 8.695 | 1.00 | 0.00 |
| ATOM | 451 | HG | SER | 1 | 471 | 36.418 | 53.035 | 9.140 | 1.00 | 0.00 |
| ATOM | 452 | N | THR | 1 | 472 | 38.386 | 56.200 | 6.149 | 1.00 | 0.00 |
| ATOM | 453 | CA | THR | 1 | 472 | 38.632 | 56.782 | 4.831 | 1.00 | 0.00 |
| ATOM | 454 | C | THR | 1 | 472 | 39.949 | 57.549 | 4.615 | 1.00 | 0.00 |
| ATOM | 455 | O | THR | 1 | 472 | 40.156 | 58.190 | 3.585 | 1.00 | 0.00 |
| ATOM | 456 | CB | THR | 1 | 472 | 37.352 | 57.555 | 4.409 | 1.00 | 0.00 |
| ATOM | 457 | OG1 | THR | 1 | 472 | 36.986 | 57.286 | 3.044 | 1.00 | 0.00 |
| ATOM | 458 | CG2 | THR | 1 | 472 | 37.389 | 59.059 | 4.709 | 1.00 | 0.00 |
| ATOM | 459 | H | THR | 1 | 472 | 37.741 | 56.694 | 6.735 | 1.00 | 0.00 |
| ATOM | 460 | HG1 | THR | 1 | 472 | 37.003 | 56.337 | 2.964 | 1.00 | 0.00 |
| ATOM | 461 | N | ILE | 1 | 473 | 40.862 | 57.437 | 5.592 | 1.00 | 0.00 |
| ATOM | 462 | CA | ILE | 1 | 473 | 42.235 | 57.795 | 5.232 | 1.00 | 0.00 |
| ATOM | 463 | C | ILE | 1 | 473 | 43.166 | 56.589 | 5.161 | 1.00 | 0.00 |
| ATOM | 464 | O | ILE | 1 | 473 | 43.824 | 56.337 | 4.160 | 1.00 | 0.00 |
| ATOM | 465 | CB | ILE | 1 | 473 | 42.764 | 58.961 | 6.084 | 1.00 | 0.00 |
| ATOM | 466 | CG1 | ILE | 1 | 473 | 44.192 | 59.367 | 5.699 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 467 | CG2 | ILE | 1 | 473 | 42.651 | 58.629 | 7.566 | 1.00 | 0.00 |
| ATOM | 468 | CD1 | ILE | 1 | 473 | 44.698 | 60.592 | 6.462 | 1.00 | 0.00 |
| ATOM | 469 | H | ILE | 1 | 473 | 40.628 | 57.026 | 6.465 | 1.00 | 0.00 |
| ATOM | 470 | N | LEU | 1 | 474 | 43.140 | 55.737 | 6.204 | 1.00 | 0.00 |
| ATOM | 471 | CA | LEU | 1 | 474 | 43.791 | 54.455 | 5.924 | 1.00 | 0.00 |
| ATOM | 472 | C | LEU | 1 | 474 | 42.834 | 53.464 | 5.287 | 1.00 | 0.00 |
| ATOM | 473 | O | LEU | 1 | 474 | 42.187 | 52.678 | 5.967 | 1.00 | 0.00 |
| ATOM | 474 | CB | LEU | 1 | 474 | 44.479 | 53.851 | 7.152 | 1.00 | 0.00 |
| ATOM | 475 | CG | LEU | 1 | 474 | 45.446 | 52.726 | 6.752 | 1.00 | 0.00 |
| ATOM | 476 | CD1 | LEU | 1 | 474 | 46.601 | 53.248 | 5.895 | 1.00 | 0.00 |
| ATOM | 477 | CD2 | LEU | 1 | 474 | 45.945 | 51.916 | 7.948 | 1.00 | 0.00 |
| ATOM | 478 | H | LEU | 1 | 474 | 42.713 | 56.012 | 7.065 | 1.00 | 0.00 |
| ATOM | 479 | N | GLY | 1 | 475 | 42.747 | 53.576 | 3.953 | 1.00 | 0.00 |
| ATOM | 480 | CA | GLY | 1 | 475 | 41.694 | 52.937 | 3.155 | 1.00 | 0.00 |
| ATOM | 481 | C | GLY | 1 | 475 | 41.140 | 51.576 | 3.568 | 1.00 | 0.00 |
| ATOM | 482 | O | GLY | 1 | 475 | 41.510 | 50.534 | 3.033 | 1.00 | 0.00 |
| ATOM | 483 | H | GLY | 1 | 475 | 43.313 | 54.312 | 3.568 | 1.00 | 0.00 |
| ATOM | 484 | N | PHE | 1 | 476 | 40.189 | 51.661 | 4.504 | 1.00 | 0.00 |
| ATOM | 485 | CA | PHE | 1 | 476 | 39.508 | 50.467 | 4.977 | 1.00 | 0.00 |
| ATOM | 486 | C | PHE | 1 | 476 | 38.024 | 50.709 | 5.165 | 1.00 | 0.00 |
| ATOM | 487 | O | PHE | 1 | 476 | 37.479 | 51.792 | 4.977 | 1.00 | 0.00 |
| ATOM | 488 | CB | PHE | 1 | 476 | 40.109 | 49.990 | 6.311 | 1.00 | 0.00 |
| ATOM | 489 | CG | PHE | 1 | 476 | 41.333 | 49.128 | 6.104 | 1.00 | 0.00 |
| ATOM | 490 | CD1 | PHE | 1 | 476 | 42.606 | 49.637 | 6.441 | 1.00 | 0.00 |
| ATOM | 491 | CD2 | PHE | 1 | 476 | 41.181 | 47.819 | 5.595 | 1.00 | 0.00 |
| ATOM | 492 | CE1 | PHE | 1 | 476 | 43.744 | 48.825 | 6.274 | 1.00 | 0.00 |
| ATOM | 493 | CE2 | PHE | 1 | 476 | 42.319 | 47.005 | 5.427 | 1.00 | 0.00 |
| ATOM | 494 | CZ | PHE | 1 | 476 | 43.588 | 47.516 | 5.772 | 1.00 | 0.00 |
| ATOM | 495 | H | PHE | 1 | 476 | 39.998 | 52.542 | 4.943 | 1.00 | 0.00 |
| ATOM | 496 | N | THR | 1 | 477 | 37.400 | 49.624 | 5.620 | 1.00 | 0.00 |
| ATOM | 497 | CA | THR | 1 | 477 | 36.155 | 49.827 | 6.326 | 1.00 | 0.00 |
| ATOM | 498 | C | THR | 1 | 477 | 36.179 | 49.050 | 7.628 | 1.00 | 0.00 |
| ATOM | 499 | O | THR | 1 | 477 | 36.128 | 47.819 | 7.665 | 1.00 | 0.00 |
| ATOM | 500 | CB | THR | 1 | 477 | 34.936 | 49.532 | 5.429 | 1.00 | 0.00 |
| ATOM | 501 | OG1 | THR | 1 | 477 | 33.732 | 49.936 | 6.097 | 1.00 | 0.00 |
| ATOM | 502 | CG2 | THR | 1 | 477 | 34.841 | 48.095 | 4.902 | 1.00 | 0.00 |
| ATOM | 503 | H | THR | 1 | 477 | 37.824 | 48.724 | 5.664 | 1.00 | 0.00 |
| ATOM | 504 | HG1 | THR | 1 | 477 | 33.555 | 49.248 | 6.740 | 1.00 | 0.00 |
| ATOM | 505 | N | TYR | 1 | 478 | 36.264 | 49.860 | 8.701 | 1.00 | 0.00 |
| ATOM | 506 | CA | TYR | 1 | 478 | 36.012 | 49.356 | 10.048 | 1.00 | 0.00 |
| ATOM | 507 | C | TYR | 1 | 478 | 34.617 | 48.753 | 10.133 | 1.00 | 0.00 |
| ATOM | 508 | O | TYR | 1 | 478 | 33.791 | 46.903 | 9.222 | 1.00 | 0.00 |
| ATOM | 509 | CB | TYR | 1 | 478 | 36.049 | 50.449 | 11.128 | 1.00 | 0.00 |
| ATOM | 510 | CG | TYR | 1 | 478 | 37.307 | 51.275 | 11.342 | 1.00 | 0.00 |
| ATOM | 511 | CD1 | TYR | 1 | 478 | 38.582 | 50.952 | 10.822 | 1.00 | 0.00 |
| ATOM | 512 | CD2 | TYR | 1 | 478 | 37.113 | 52.423 | 12.130 | 1.00 | 0.00 |
| ATOM | 513 | CE1 | TYR | 1 | 478 | 39.665 | 51.822 | 11.087 | 1.00 | 0.00 |
| ATOM | 514 | CE2 | TYR | 1 | 478 | 38.183 | 53.278 | 12.404 | 1.00 | 0.00 |
| ATOM | 515 | CZ | TYR | 1 | 478 | 39.448 | 52.979 | 11.873 | 1.00 | 0.00 |
| ATOM | 516 | OH | TYR | 1 | 478 | 40.479 | 53.871 | 12.155 | 1.00 | 0.00 |
| ATOM | 517 | H | TYR | 1 | 478 | 36.289 | 50.853 | 8.591 | 1.00 | 0.00 |
| ATOM | 518 | HH | TYR | 1 | 478 | 40.091 | 54.550 | 12.720 | 1.00 | 0.00 |
| ATOM | 519 | N | GLU | 1 | 479 | 34.423 | 48.052 | 11.254 | 1.00 | 0.00 |
| ATOM | 520 | CA | GLU | 1 | 479 | 33.132 | 47.420 | 11.434 | 1.00 | 0.00 |
| ATOM | 521 | C | GLU | 1 | 479 | 32.405 | 47.978 | 12.627 | 1.00 | 0.00 |
| ATOM | 522 | O | GLU | 1 | 479 | 32.655 | 47.672 | 13.795 | 1.00 | 0.00 |
| ATOM | 523 | CB | GLU | 1 | 479 | 33.235 | 45.899 | 11.487 | 1.00 | 0.00 |
| ATOM | 524 | CG | GLU | 1 | 479 | 31.895 | 45.241 | 11.144 | 1.00 | 0.00 |
| ATOM | 525 | CD | GLU | 1 | 479 | 31.616 | 45.311 | 9.653 | 1.00 | 0.00 |
| ATOM | 526 | OE1 | GLU | 1 | 479 | 31.570 | 46.394 | 9.076 | 1.00 | 0.00 |
| ATOM | 527 | OE2 | GLU | 1 | 479 | 31.453 | 44.256 | 9.055 | 1.00 | 0.00 |
| ATOM | 528 | H | GLU | 1 | 479 | 35.076 | 48.036 | 12.012 | 1.00 | 0.00 |
| ATOM | 529 | N | ILE | 1 | 480 | 31.493 | 48.900 | 12.265 | 1.00 | 0.00 |
| ATOM | 530 | CA | ILE | 1 | 480 | 30.654 | 49.499 | 13.306 | 1.00 | 0.00 |
| ATOM | 531 | C | ILE | 1 | 480 | 29.576 | 48.548 | 13.793 | 1.00 | 0.00 |
| ATOM | 532 | O | ILE | 1 | 480 | 28.825 | 47.963 | 12.996 | 1.00 | 0.00 |
| ATOM | 533 | CB | ILE | 1 | 480 | 30.115 | 50.881 | 12.898 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 534 | CG1 | ILE | 1 | 480 | 29.472 | 51.582 | 14.098 | 1.00 | 0.00 |
| ATOM | 535 | CG2 | ILE | 1 | 480 | 29.160 | 50.809 | 11.698 | 1.00 | 0.00 |
| ATOM | 536 | CD1 | ILE | 1 | 480 | 29.278 | 53.079 | 13.888 | 1.00 | 0.00 |
| ATOM | 537 | H | ILE | 1 | 480 | 31.368 | 49.103 | 11.294 | 1.00 | 0.00 |
| ATOM | 538 | N | ARG | 1 | 481 | 29.593 | 48.312 | 15.098 | 1.00 | 0.00 |
| ATOM | 539 | CA | ARG | 1 | 481 | 29.201 | 46.992 | 15.554 | 1.00 | 0.00 |
| ATOM | 540 | C | ARG | 1 | 481 | 29.189 | 46.981 | 17.060 | 1.00 | 0.00 |
| ATOM | 541 | O | ARG | 1 | 481 | 29.570 | 47.936 | 17.743 | 1.00 | 0.00 |
| ATOM | 542 | CB | ARG | 1 | 481 | 30.224 | 45.967 | 15.048 | 1.00 | 0.00 |
| ATOM | 543 | CG | ARG | 1 | 481 | 29.695 | 44.575 | 14.726 | 1.00 | 0.00 |
| ATOM | 544 | CD | ARG | 1 | 481 | 30.859 | 43.657 | 14.383 | 1.00 | 0.00 |
| ATOM | 545 | NE | ARG | 1 | 481 | 30.388 | 42.306 | 14.120 | 1.00 | 0.00 |
| ATOM | 546 | CZ | ARG | 1 | 481 | 31.213 | 41.365 | 13.628 | 1.00 | 0.00 |
| ATOM | 547 | NH1 | ARG | 1 | 481 | 30.726 | 40.150 | 13.442 | 1.00 | 0.00 |
| ATOM | 548 | NH2 | ARG | 1 | 481 | 32.478 | 41.637 | 13.320 | 1.00 | 0.00 |
| ATOM | 549 | H | ARG | 1 | 481 | 30.106 | 48.909 | 15.709 | 1.00 | 0.00 |
| ATOM | 550 | HE | ARG | 1 | 481 | 29.419 | 42.107 | 14.290 | 1.00 | 0.00 |
| ATOM | 551 | 1HH1 | ARG | 1 | 481 | 31.308 | 39.432 | 13.047 | 1.00 | 0.00 |
| ATOM | 552 | 2HH1 | ARG | 1 | 481 | 29.791 | 39.904 | 13.688 | 1.00 | 0.00 |
| ATOM | 553 | 1HH2 | ARG | 1 | 481 | 33.096 | 40.896 | 12.993 | 1.00 | 0.00 |
| ATOM | 554 | 2HH2 | ARG | 1 | 481 | 32.914 | 42.531 | 13.423 | 1.00 | 0.00 |
| ATOM | 555 | N | LEU | 1 | 482 | 28.778 | 45.813 | 17.565 | 1.00 | 0.00 |
| ATOM | 556 | CA | LEU | 1 | 482 | 29.324 | 45.280 | 18.809 | 1.00 | 0.00 |
| ATOM | 557 | C | LEU | 1 | 482 | 29.353 | 43.786 | 18.608 | 1.00 | 0.00 |
| ATOM | 558 | O | LEU | 1 | 482 | 28.469 | 43.290 | 17.904 | 1.00 | 0.00 |
| ATOM | 559 | CB | LEU | 1 | 482 | 28.450 | 45.621 | 20.032 | 1.00 | 0.00 |
| ATOM | 560 | CG | LEU | 1 | 482 | 26.989 | 45.126 | 20.087 | 1.00 | 0.00 |
| ATOM | 561 | CD1 | LEU | 1 | 482 | 26.470 | 45.124 | 21.525 | 1.00 | 0.00 |
| ATOM | 562 | CD2 | LEU | 1 | 482 | 26.025 | 45.895 | 19.178 | 1.00 | 0.00 |
| ATOM | 563 | H | LEU | 1 | 482 | 28.335 | 45.171 | 16.937 | 1.00 | 0.00 |
| ATOM | 564 | N | VAL | 1 | 483 | 30.285 | 43.080 | 19.260 | 1.00 | 0.00 |
| ATOM | 565 | CA | VAL | 1 | 483 | 29.796 | 41.738 | 19.584 | 1.00 | 0.00 |
| ATOM | 566 | C | VAL | 1 | 483 | 28.855 | 41.771 | 20.789 | 1.00 | 0.00 |
| ATOM | 567 | O | VAL | 1 | 483 | 27.666 | 41.447 | 20.711 | 1.00 | 0.00 |
| ATOM | 568 | CB | VAL | 1 | 483 | 30.937 | 40.703 | 19.685 | 1.00 | 0.00 |
| ATOM | 569 | CG1 | VAL | 1 | 483 | 31.448 | 40.394 | 18.275 | 1.00 | 0.00 |
| ATOM | 570 | CG2 | VAL | 1 | 483 | 32.097 | 41.098 | 20.608 | 1.00 | 0.00 |
| ATOM | 571 | H | VAL | 1 | 483 | 31.081 | 43.515 | 19.678 | 1.00 | 0.00 |
| ATOM | 572 | N | GLU | 1 | 484 | 29.420 | 42.325 | 21.873 | 1.00 | 0.00 |
| ATOM | 573 | CA | GLU | 1 | 484 | 28.659 | 42.547 | 23.092 | 1.00 | 0.00 |
| ATOM | 574 | C | GLU | 1 | 484 | 29.310 | 43.705 | 23.841 | 1.00 | 0.00 |
| ATOM | 575 | O | GLU | 1 | 484 | 30.430 | 44.090 | 23.506 | 1.00 | 0.00 |
| ATOM | 576 | CB | GLU | 1 | 484 | 28.565 | 41.223 | 23.869 | 1.00 | 0.00 |
| ATOM | 577 | CG | GLU | 1 | 484 | 27.221 | 40.972 | 24.575 | 1.00 | 0.00 |
| ATOM | 578 | CD | GLU | 1 | 484 | 27.083 | 39.502 | 24.958 | 1.00 | 0.00 |
| ATOM | 579 | OE1 | GLU | 1 | 484 | 26.700 | 38.706 | 24.109 | 1.00 | 0.00 |
| ATOM | 580 | OE2 | GLU | 1 | 484 | 27.343 | 39.132 | 26.100 | 1.00 | 0.00 |
| ATOM | 581 | H | GLU | 1 | 484 | 30.378 | 42.598 | 21.843 | 1.00 | 0.00 |
| ATOM | 582 | N | ASP | 1 | 485 | 28.527 | 44.253 | 24.801 | 1.00 | 0.00 |
| ATOM | 583 | CA | ASP | 1 | 485 | 28.693 | 45.553 | 25.483 | 1.00 | 0.00 |
| ATOM | 584 | C | ASP | 1 | 485 | 30.040 | 46.252 | 25.399 | 1.00 | 0.00 |
| ATOM | 585 | O | ASP | 1 | 485 | 31.109 | 45.661 | 25.535 | 1.00 | 0.00 |
| ATOM | 586 | CB | ASP | 1 | 485 | 28.207 | 45.410 | 26.944 | 1.00 | 0.00 |
| ATOM | 587 | CG | ASP | 1 | 485 | 28.305 | 46.687 | 27.774 | 1.00 | 0.00 |
| ATOM | 588 | OD1 | ASP | 1 | 485 | 27.339 | 47.420 | 27.903 | 1.00 | 0.00 |
| ATOM | 589 | OD2 | ASP | 1 | 485 | 29.356 | 46.978 | 28.318 | 1.00 | 0.00 |
| ATOM | 590 | H | ASP | 1 | 485 | 27.751 | 43.694 | 25.090 | 1.00 | 0.00 |
| ATOM | 591 | N | GLY | 1 | 486 | 29.958 | 47.577 | 25.177 | 1.00 | 0.00 |
| ATOM | 592 | CA | GLY | 1 | 486 | 31.196 | 48.353 | 25.037 | 1.00 | 0.00 |
| ATOM | 593 | C | GLY | 1 | 486 | 32.144 | 48.470 | 26.235 | 1.00 | 0.00 |
| ATOM | 594 | O | GLY | 1 | 486 | 33.150 | 49.189 | 26.190 | 1.00 | 0.00 |
| ATOM | 595 | H | GLY | 1 | 486 | 29.038 | 47.969 | 25.096 | 1.00 | 0.00 |
| ATOM | 596 | N | LYS | 1 | 487 | 31.804 | 47.767 | 27.323 | 1.00 | 0.00 |
| ATOM | 597 | CA | LYS | 1 | 487 | 32.516 | 47.906 | 28.597 | 1.00 | 0.00 |
| ATOM | 598 | C | LYS | 1 | 487 | 32.823 | 46.581 | 29.274 | 1.00 | 0.00 |
| ATOM | 599 | O | LYS | 1 | 487 | 33.950 | 46.367 | 29.718 | 1.00 | 0.00 |
| ATOM | 600 | CB | LYS | 1 | 487 | 31.753 | 48.812 | 29.569 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 601 | CG | LYS | 1 | 487 | 31.429 | 50.195 | 29.000 | 1.00 | 0.00 |
| ATOM | 602 | CD | LYS | 1 | 487 | 30.321 | 50.911 | 29.770 | 1.00 | 0.00 |
| ATOM | 603 | CE | LYS | 1 | 487 | 29.033 | 50.084 | 29.858 | 1.00 | 0.00 |
| ATOM | 604 | NZ | LYS | 1 | 487 | 28.576 | 49.683 | 28.528 | 1.00 | 0.00 |
| ATOM | 605 | H | LYS | 1 | 487 | 30.993 | 47.193 | 27.248 | 1.00 | 0.00 |
| ATOM | 606 | 1HZ | LYS | 1 | 487 | 29.049 | 50.212 | 27.773 | 1.00 | 0.00 |
| ATOM | 607 | 2HZ | LYS | 1 | 487 | 28.690 | 48.659 | 28.373 | 1.00 | 0.00 |
| ATOM | 608 | 3HZ | LYS | 1 | 487 | 27.571 | 49.907 | 28.420 | 1.00 | 0.00 |
| ATOM | 609 | N | TYR | 1 | 488 | 31.801 | 45.687 | 29.290 | 1.00 | 0.00 |
| ATOM | 610 | CA | TYR | 1 | 488 | 32.098 | 44.313 | 29.699 | 1.00 | 0.00 |
| ATOM | 611 | C | TYR | 1 | 488 | 32.845 | 43.551 | 28.615 | 1.00 | 0.00 |
| ATOM | 612 | O | TYR | 1 | 488 | 33.699 | 42.709 | 28.896 | 1.00 | 0.00 |
| ATOM | 613 | CB | TYR | 1 | 488 | 30.827 | 43.563 | 30.208 | 1.00 | 0.00 |
| ATOM | 614 | CG | TYR | 1 | 488 | 30.419 | 42.415 | 29.296 | 1.00 | 0.00 |
| ATOM | 615 | CD1 | TYR | 1 | 488 | 29.657 | 42.709 | 28.153 | 1.00 | 0.00 |
| ATOM | 616 | CD2 | TYR | 1 | 488 | 30.878 | 41.104 | 29.557 | 1.00 | 0.00 |
| ATOM | 617 | CE1 | TYR | 1 | 488 | 29.528 | 41.738 | 27.152 | 1.00 | 0.00 |
| ATOM | 618 | CE2 | TYR | 1 | 488 | 30.730 | 40.121 | 28.558 | 1.00 | 0.00 |
| ATOM | 619 | CZ | TYR | 1 | 488 | 30.136 | 40.481 | 27.329 | 1.00 | 0.00 |
| ATOM | 620 | OH | TYR | 1 | 488 | 30.170 | 39.619 | 26.243 | 1.00 | 0.00 |
| ATOM | 621 | H | TYR | 1 | 488 | 30.930 | 45.872 | 28.828 | 1.00 | 0.00 |
| ATOM | 622 | HH | TYR | 1 | 488 | 29.339 | 39.128 | 26.277 | 1.00 | 0.00 |
| ATOM | 623 | N | GLY | 1 | 489 | 32.461 | 43.883 | 27.363 | 1.00 | 0.00 |
| ATOM | 624 | CA | GLY | 1 | 489 | 33.021 | 43.175 | 26.218 | 1.00 | 0.00 |
| ATOM | 625 | C | GLY | 1 | 489 | 34.260 | 43.800 | 25.616 | 1.00 | 0.00 |
| ATOM | 626 | O | GLY | 1 | 489 | 34.459 | 43.791 | 24.406 | 1.00 | 0.00 |
| ATOM | 627 | H | GLY | 1 | 489 | 31.769 | 44.597 | 27.232 | 1.00 | 0.00 |
| ATOM | 628 | N | ALA | 1 | 490 | 35.123 | 44.278 | 26.531 | 1.00 | 0.00 |
| ATOM | 629 | CA | ALA | 1 | 490 | 36.490 | 44.601 | 26.091 | 1.00 | 0.00 |
| ATOM | 630 | C | ALA | 1 | 490 | 37.401 | 43.374 | 25.963 | 1.00 | 0.00 |
| ATOM | 631 | O | ALA | 1 | 490 | 38.575 | 43.402 | 25.576 | 1.00 | 0.00 |
| ATOM | 632 | CB | ALA | 1 | 490 | 37.125 | 45.592 | 27.066 | 1.00 | 0.00 |
| ATOM | 633 | H | ALA | 1 | 490 | 34.909 | 44.177 | 27.505 | 1.00 | 0.00 |
| ATOM | 634 | N | GLN | 1 | 491 | 36.772 | 42.230 | 26.327 | 1.00 | 0.00 |
| ATOM | 635 | CA | GLN | 1 | 491 | 37.344 | 40.882 | 26.253 | 1.00 | 0.00 |
| ATOM | 636 | C | GLN | 1 | 491 | 37.960 | 40.430 | 24.932 | 1.00 | 0.00 |
| ATOM | 637 | O | GLN | 1 | 491 | 38.601 | 39.384 | 24.869 | 1.00 | 0.00 |
| ATOM | 638 | CB | GLN | 1 | 491 | 36.250 | 39.897 | 26.684 | 1.00 | 0.00 |
| ATOM | 639 | CG | GLN | 1 | 491 | 35.097 | 39.821 | 25.669 | 1.00 | 0.00 |
| ATOM | 640 | CD | GLN | 1 | 491 | 33.853 | 39.260 | 26.319 | 1.00 | 0.00 |
| ATOM | 641 | OE1 | GLN | 1 | 491 | 33.236 | 39.876 | 27.180 | 1.00 | 0.00 |
| ATOM | 642 | NE2 | GLN | 1 | 491 | 33.467 | 38.075 | 25.865 | 1.00 | 0.00 |
| ATOM | 643 | H | GLN | 1 | 491 | 35.831 | 42.334 | 26.641 | 1.00 | 0.00 |
| ATOM | 644 | 1HE2 | GLN | 1 | 491 | 32.684 | 37.612 | 26.280 | 1.00 | 0.00 |
| ATOM | 645 | 2HE2 | GLN | 1 | 491 | 33.986 | 37.750 | 25.076 | 1.00 | 0.00 |
| ATOM | 646 | N | ASP | 1 | 492 | 37.667 | 41.211 | 23.883 | 1.00 | 0.00 |
| ATOM | 647 | CA | ASP | 1 | 492 | 38.033 | 40.828 | 22.524 | 1.00 | 0.00 |
| ATOM | 648 | C | ASP | 1 | 492 | 39.495 | 40.469 | 22.323 | 1.00 | 0.00 |
| ATOM | 649 | O | ASP | 1 | 492 | 39.848 | 39.368 | 21.902 | 1.00 | 0.00 |
| ATOM | 650 | CB | ASP | 1 | 492 | 37.606 | 41.963 | 21.591 | 1.00 | 0.00 |
| ATOM | 651 | CG | ASP | 1 | 492 | 37.921 | 41.652 | 20.143 | 1.00 | 0.00 |
| ATOM | 652 | OD1 | ASP | 1 | 492 | 37.066 | 41.118 | 19.454 | 1.00 | 0.00 |
| ATOM | 653 | OD2 | ASP | 1 | 492 | 39.015 | 41.965 | 19.676 | 1.00 | 0.00 |
| ATOM | 654 | H | ASP | 1 | 492 | 37.221 | 43.091 | 24.021 | 1.00 | 0.00 |
| ATOM | 655 | N | ASP | 1 | 493 | 40.338 | 41.475 | 22.627 | 1.00 | 0.00 |
| ATOM | 656 | CA | ASP | 1 | 493 | 41.707 | 41.500 | 22.081 | 1.00 | 0.00 |
| ATOM | 657 | C | ASP | 1 | 493 | 42.532 | 40.224 | 22.128 | 1.00 | 0.00 |
| ATOM | 658 | O | ASP | 1 | 493 | 42.669 | 39.505 | 21.132 | 1.00 | 0.00 |
| ATOM | 659 | CB | ASP | 1 | 493 | 42.513 | 42.695 | 22.628 | 1.00 | 0.00 |
| ATOM | 660 | CG | ASP | 1 | 493 | 43.799 | 42.889 | 21.826 | 1.00 | 0.00 |
| ATOM | 661 | OD1 | ASP | 1 | 493 | 43.776 | 42.763 | 20.614 | 1.00 | 0.00 |
| ATOM | 662 | OD2 | ASP | 1 | 493 | 44.842 | 43.151 | 22.399 | 1.00 | 0.00 |
| ATOM | 663 | H | ASP | 1 | 493 | 39.869 | 42.306 | 22.916 | 1.00 | 0.00 |
| ATOM | 664 | N | VAL | 1 | 494 | 43.062 | 39.967 | 23.336 | 1.00 | 0.00 |
| ATOM | 665 | CA | VAL | 1 | 494 | 43.909 | 38.790 | 23.520 | 1.00 | 0.00 |
| ATOM | 666 | C | VAL | 1 | 494 | 43.119 | 37.501 | 23.335 | 1.00 | 0.00 |
| ATOM | 667 | O | VAL | 1 | 494 | 43.628 | 36.421 | 23.051 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 668 | CB | VAL | 1 | 494 | 44.595 | 38.852 | 24.897 | 1.00 | 0.00 |
| ATOM | 669 | CG1 | VAL | 1 | 494 | 45.603 | 37.717 | 25.112 | 1.00 | 0.00 |
| ATOM | 670 | CG2 | VAL | 1 | 494 | 45.262 | 40.215 | 25.105 | 1.00 | 0.00 |
| ATOM | 671 | H | VAL | 1 | 494 | 42.754 | 40.533 | 24.094 | 1.00 | 0.00 |
| ATOM | 672 | N | ASN | 1 | 495 | 41.797 | 37.655 | 23.480 | 1.00 | 0.00 |
| ATOM | 673 | CA | ASN | 1 | 495 | 40.938 | 36.508 | 23.173 | 1.00 | 0.00 |
| ATOM | 674 | C | ASN | 1 | 495 | 40.918 | 36.093 | 21.702 | 1.00 | 0.00 |
| ATOM | 675 | O | ASN | 1 | 495 | 40.667 | 34.941 | 21.341 | 1.00 | 0.00 |
| ATOM | 676 | CB | ASN | 1 | 495 | 39.532 | 36.745 | 23.723 | 1.00 | 0.00 |
| ATOM | 677 | CG | ASN | 1 | 495 | 38.751 | 35.459 | 23.700 | 1.00 | 0.00 |
| ATOM | 678 | OD1 | ASN | 1 | 495 | 38.966 | 34.551 | 24.500 | 1.00 | 0.00 |
| ATOM | 679 | ND2 | ASN | 1 | 495 | 37.900 | 35.374 | 22.681 | 1.00 | 0.00 |
| ATOM | 680 | H | ASN | 1 | 495 | 41.450 | 38.590 | 23.590 | 1.00 | 0.00 |
| ATOM | 681 | 1HD2 | ASN | 1 | 495 | 37.473 | 34.502 | 22.451 | 1.00 | 0.00 |
| ATOM | 682 | 2HD2 | ASN | 1 | 495 | 37.737 | 36.196 | 22.137 | 1.00 | 0.00 |
| ATOM | 683 | N | GLY | 1 | 496 | 41.252 | 37.069 | 20.859 | 1.00 | 0.00 |
| ATOM | 684 | CA | GLY | 1 | 496 | 41.492 | 36.632 | 19.503 | 1.00 | 0.00 |
| ATOM | 685 | C | GLY | 1 | 496 | 42.950 | 36.423 | 19.187 | 1.00 | 0.00 |
| ATOM | 686 | O | GLY | 1 | 496 | 43.426 | 36.872 | 18.156 | 1.00 | 0.00 |
| ATOM | 687 | H | GLY | 1 | 496 | 41.434 | 38.000 | 21.167 | 1.00 | 0.00 |
| ATOM | 688 | N | GLN | 1 | 497 | 43.653 | 35.691 | 20.067 | 1.00 | 0.00 |
| ATOM | 689 | CA | GLN | 1 | 497 | 44.992 | 35.197 | 19.702 | 1.00 | 0.00 |
| ATOM | 690 | C | GLN | 1 | 497 | 45.079 | 34.517 | 18.339 | 1.00 | 0.00 |
| ATOM | 691 | O | GLN | 1 | 497 | 46.094 | 34.507 | 17.654 | 1.00 | 0.00 |
| ATOM | 692 | CB | GLN | 1 | 497 | 45.480 | 34.166 | 20.712 | 1.00 | 0.00 |
| ATOM | 693 | CG | GLN | 1 | 497 | 45.906 | 34.705 | 22.071 | 1.00 | 0.00 |
| ATOM | 694 | CD | GLN | 1 | 497 | 46.059 | 33.533 | 23.013 | 1.00 | 0.00 |
| ATOM | 695 | OE1 | GLN | 1 | 497 | 45.681 | 32.405 | 22.722 | 1.00 | 0.00 |
| ATOM | 696 | NE2 | GLN | 1 | 497 | 46.656 | 33.835 | 24.170 | 1.00 | 0.00 |
| ATOM | 697 | H | GLN | 1 | 497 | 43.214 | 35.515 | 20.948 | 1.00 | 0.00 |
| ATOM | 698 | 1HE2 | GLN | 1 | 497 | 46.856 | 33.098 | 24.813 | 1.00 | 0.00 |
| ATOM | 699 | 2HE2 | GLN | 1 | 497 | 46.862 | 34.791 | 24.370 | 1.00 | 0.00 |
| ATOM | 700 | N | TRP | 1 | 498 | 43.962 | 33.863 | 18.024 | 1.00 | 0.00 |
| ATOM | 701 | CA | TRP | 1 | 498 | 43.735 | 33.396 | 16.665 | 1.00 | 0.00 |
| ATOM | 702 | C | TRP | 1 | 498 | 42.494 | 34.118 | 16.183 | 1.00 | 0.00 |
| ATOM | 703 | O | TRP | 1 | 498 | 42.570 | 35.221 | 15.652 | 1.00 | 0.00 |
| ATOM | 704 | CB | TRP | 1 | 498 | 43.708 | 31.850 | 16.557 | 1.00 | 0.00 |
| ATOM | 705 | CG | TRP | 1 | 498 | 43.126 | 31.126 | 17.762 | 1.00 | 0.00 |
| ATOM | 706 | CD1 | TRP | 1 | 498 | 43.717 | 30.982 | 19.028 | 1.00 | 0.00 |
| ATOM | 707 | CD2 | TRP | 1 | 498 | 41.881 | 30.396 | 17.854 | 1.00 | 0.00 |
| ATOM | 708 | NE1 | TRP | 1 | 498 | 42.947 | 30.239 | 19.864 | 1.00 | 0.00 |
| ATOM | 709 | CE2 | TRP | 1 | 498 | 41.800 | 29.850 | 19.181 | 1.00 | 0.00 |
| ATOM | 710 | CE3 | TRP | 1 | 498 | 40.837 | 30.155 | 16.936 | 1.00 | 0.00 |
| ATOM | 711 | CZ2 | TRP | 1 | 498 | 40.683 | 29.076 | 19.659 | 1.00 | 0.00 |
| ATOM | 712 | CZ3 | TRP | 1 | 498 | 39.724 | 29.381 | 17.328 | 1.00 | 0.00 |
| ATOM | 713 | CH2 | TRP | 1 | 498 | 39.647 | 28.843 | 18.631 | 1.00 | 0.00 |
| ATOM | 714 | H | TRP | 1 | 498 | 43.137 | 33.943 | 18.646 | 1.00 | 0.00 |
| ATOM | 715 | HE1 | TRP | 1 | 498 | 43.187 | 30.035 | 20.795 | 1.00 | 0.00 |
| ATOM | 716 | N | ASN | 1 | 499 | 41.339 | 33.527 | 16.487 | 1.00 | 0.00 |
| ATOM | 717 | CA | ASN | 1 | 499 | 40.160 | 34.369 | 16.667 | 1.00 | 0.00 |
| ATOM | 718 | C | ASN | 1 | 499 | 39.188 | 33.619 | 17.527 | 1.00 | 0.00 |
| ATOM | 719 | O | ASN | 1 | 499 | 38.184 | 33.095 | 17.054 | 1.00 | 0.00 |
| ATOM | 720 | CB | ASN | 1 | 499 | 39.501 | 34.881 | 15.360 | 1.00 | 0.00 |
| ATOM | 721 | CG | ASN | 1 | 499 | 39.552 | 33.944 | 14.158 | 1.00 | 0.00 |
| ATOM | 722 | OD1 | ASN | 1 | 499 | 40.038 | 34.322 | 13.089 | 1.00 | 0.00 |
| ATOM | 723 | ND2 | ASN | 1 | 499 | 39.013 | 32.735 | 14.345 | 1.00 | 0.00 |
| ATOM | 724 | H | ASN | 1 | 499 | 41.300 | 32.545 | 16.643 | 1.00 | 0.00 |
| ATOM | 725 | 1HD2 | ASN | 1 | 499 | 39.053 | 32.064 | 13.607 | 1.00 | 0.00 |
| ATOM | 726 | 2HD2 | ASN | 1 | 499 | 38.577 | 32.508 | 15.215 | 1.00 | 0.00 |
| ATOM | 727 | N | GLY | 1 | 500 | 39.576 | 33.484 | 18.808 | 1.00 | 0.00 |
| ATOM | 728 | CA | GLY | 1 | 500 | 38.872 | 32.488 | 19.614 | 1.00 | 0.00 |
| ATOM | 729 | C | GLY | 1 | 500 | 39.227 | 32.400 | 21.090 | 1.00 | 0.00 |
| ATOM | 730 | O | GLY | 1 | 500 | 38.432 | 32.778 | 21.940 | 1.00 | 0.00 |
| ATOM | 731 | H | GLY | 1 | 500 | 40.282 | 34.058 | 19.231 | 1.00 | 0.00 |
| ATOM | 732 | N | MET | 1 | 501 | 40.429 | 31.845 | 21.360 | 1.00 | 0.00 |
| ATOM | 733 | CA | MET | 1 | 501 | 40.922 | 31.555 | 22.720 | 1.00 | 0.00 |
| ATOM | 734 | C | MET | 1 | 501 | 39.997 | 30.865 | 23.727 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 735 | O | MET | 1 | 501 | 40.193 | 29.692 | 24.041 | 1.00 | 0.00 |
| ATOM | 736 | CB | MET | 1 | 501 | 41.639 | 32.755 | 23.351 | 1.00 | 0.00 |
| ATOM | 737 | CG | MET | 1 | 501 | 42.612 | 32.348 | 24.463 | 1.00 | 0.00 |
| ATOM | 738 | SD | MET | 1 | 501 | 43.389 | 33.750 | 25.283 | 1.00 | 0.00 |
| ATOM | 739 | CE | MET | 1 | 501 | 41.941 | 34.364 | 26.158 | 1.00 | 0.00 |
| ATOM | 740 | H | MET | 1 | 501 | 41.019 | 31.651 | 20.580 | 1.00 | 0.00 |
| ATOM | 741 | N | VAL | 1 | 502 | 39.000 | 31.604 | 24.240 | 1.00 | 0.00 |
| ATOM | 742 | CA | VAL | 1 | 502 | 37.990 | 30.868 | 24.993 | 1.00 | 0.00 |
| ATOM | 743 | C | VAL | 1 | 502 | 36.842 | 30.363 | 24.133 | 1.00 | 0.00 |
| ATOM | 744 | O | VAL | 1 | 502 | 36.289 | 29.293 | 24.375 | 1.00 | 0.00 |
| ATOM | 745 | CB | VAL | 1 | 502 | 37.492 | 31.642 | 26.230 | 1.00 | 0.00 |
| ATOM | 746 | CG1 | VAL | 1 | 502 | 38.670 | 31.961 | 27.152 | 1.00 | 0.00 |
| ATOM | 747 | CG2 | VAL | 1 | 502 | 36.660 | 32.888 | 25.906 | 1.00 | 0.00 |
| ATOM | 748 | H | VAL | 1 | 502 | 38.894 | 32.564 | 23.966 | 1.00 | 0.00 |
| ATOM | 749 | N | ARG | 1 | 503 | 36.511 | 31.181 | 23.130 | 1.00 | 0.00 |
| ATOM | 750 | CA | ARG | 1 | 503 | 35.560 | 30.742 | 22.119 | 1.00 | 0.00 |
| ATOM | 751 | C | ARG | 1 | 503 | 36.250 | 29.974 | 21.011 | 1.00 | 0.00 |
| ATOM | 752 | O | ARG | 1 | 503 | 37.450 | 29.706 | 21.045 | 1.00 | 0.00 |
| ATOM | 753 | CB | ARG | 1 | 503 | 34.785 | 31.946 | 21.581 | 1.00 | 0.00 |
| ATOM | 754 | CG | ARG | 1 | 503 | 33.651 | 32.375 | 22.513 | 1.00 | 0.00 |
| ATOM | 755 | CD | ARG | 1 | 503 | 32.249 | 31.999 | 22.012 | 1.00 | 0.00 |
| ATOM | 756 | NE | ARG | 1 | 503 | 32.045 | 30.554 | 21.856 | 1.00 | 0.00 |
| ATOM | 757 | CZ | ARG | 1 | 503 | 30.929 | 29.938 | 22.298 | 1.00 | 0.00 |
| ATOM | 758 | NH1 | ARG | 1 | 503 | 30.743 | 28.655 | 22.023 | 1.00 | 0.00 |
| ATOM | 759 | NH2 | ARG | 1 | 503 | 30.016 | 30.608 | 23.001 | 1.00 | 0.00 |
| ATOM | 760 | H | ARG | 1 | 503 | 37.035 | 32.018 | 22.980 | 1.00 | 0.00 |
| ATOM | 761 | HE | ARG | 1 | 503 | 32.700 | 30.031 | 21.293 | 1.00 | 0.00 |
| ATOM | 762 | 1HH1 | ARG | 1 | 503 | 29.942 | 28.132 | 22.303 | 1.00 | 0.00 |
| ATOM | 763 | 2HH1 | ARG | 1 | 503 | 31.462 | 28.169 | 21.495 | 1.00 | 0.00 |
| ATOM | 764 | 1HH2 | ARG | 1 | 503 | 29.198 | 30.142 | 23.340 | 1.00 | 0.00 |
| ATOM | 765 | 2HH2 | ARG | 1 | 503 | 30.135 | 31.580 | 23.206 | 1.00 | 0.00 |
| ATOM | 766 | N | GLU | 1 | 504 | 35.406 | 29.583 | 20.051 | 1.00 | 0.00 |
| ATOM | 767 | CA | GLU | 1 | 504 | 35.890 | 28.882 | 18.870 | 1.00 | 0.00 |
| ATOM | 768 | C | GLU | 1 | 504 | 36.237 | 29.908 | 17.803 | 1.00 | 0.00 |
| ATOM | 769 | O | GLU | 1 | 504 | 36.469 | 31.070 | 18.132 | 1.00 | 0.00 |
| ATOM | 770 | CB | GLU | 1 | 504 | 34.830 | 27.877 | 18.387 | 1.00 | 0.00 |
| ATOM | 771 | CG | GLU | 1 | 504 | 34.242 | 26.925 | 19.445 | 1.00 | 0.00 |
| ATOM | 772 | CD | GLU | 1 | 504 | 33.187 | 27.613 | 20.300 | 1.00 | 0.00 |
| ATOM | 773 | OE1 | GLU | 1 | 504 | 33.185 | 27.455 | 21.510 | 1.00 | 0.00 |
| ATOM | 774 | OE2 | GLU | 1 | 504 | 32.342 | 28.322 | 19.776 | 1.00 | 0.00 |
| ATOM | 775 | H | GLU | 1 | 504 | 34.459 | 29.896 | 20.064 | 1.00 | 0.00 |
| ATOM | 776 | N | LEU | 1 | 505 | 36.223 | 29.466 | 16.528 | 1.00 | 0.00 |
| ATOM | 777 | CA | LEU | 1 | 505 | 36.388 | 30.394 | 15.404 | 1.00 | 0.00 |
| ATOM | 778 | C | LEU | 1 | 505 | 35.285 | 31.441 | 15.301 | 1.00 | 0.00 |
| ATOM | 779 | O | LEU | 1 | 505 | 34.352 | 31.333 | 14.505 | 1.00 | 0.00 |
| ATOM | 780 | CB | LEU | 1 | 505 | 36.464 | 29.611 | 14.090 | 1.00 | 0.00 |
| ATOM | 781 | CG | LEU | 1 | 505 | 37.611 | 28.602 | 13.994 | 1.00 | 0.00 |
| ATOM | 782 | CD1 | LEU | 1 | 505 | 37.354 | 27.567 | 12.899 | 1.00 | 0.00 |
| ATOM | 783 | CD2 | LEU | 1 | 505 | 38.968 | 29.281 | 13.811 | 1.00 | 0.00 |
| ATOM | 784 | H | LEU | 1 | 505 | 36.120 | 28.498 | 16.343 | 1.00 | 0.00 |
| ATOM | 785 | N | ILE | 1 | 506 | 35.429 | 32.452 | 16.163 | 1.00 | 0.00 |
| ATOM | 786 | CA | ILE | 1 | 506 | 34.503 | 33.575 | 16.182 | 1.00 | 0.00 |
| ATOM | 787 | C | ILE | 1 | 506 | 35.132 | 34.672 | 15.342 | 1.00 | 0.00 |
| ATOM | 788 | O | ILE | 1 | 506 | 36.293 | 34.553 | 14.981 | 1.00 | 0.00 |
| ATOM | 789 | CB | ILE | 1 | 506 | 34.240 | 33.971 | 17.654 | 1.00 | 0.00 |
| ATOM | 790 | CG1 | ILE | 1 | 506 | 33.018 | 34.878 | 17.845 | 1.00 | 0.00 |
| ATOM | 791 | CG2 | ILE | 1 | 506 | 35.491 | 34.581 | 18.308 | 1.00 | 0.00 |
| ATOM | 792 | CD1 | ILE | 1 | 506 | 32.701 | 35.170 | 19.313 | 1.00 | 0.00 |
| ATOM | 793 | H | ILE | 1 | 506 | 36.252 | 32.443 | 16.735 | 1.00 | 0.00 |
| ATOM | 794 | N | ASP | 1 | 507 | 34.351 | 35.708 | 15.033 | 1.00 | 0.00 |
| ATOM | 795 | CA | ASP | 1 | 507 | 34.816 | 36.858 | 14.249 | 1.00 | 0.00 |
| ATOM | 796 | C | ASP | 1 | 507 | 36.113 | 37.526 | 14.747 | 1.00 | 0.00 |
| ATOM | 797 | O | ASP | 1 | 507 | 37.209 | 37.327 | 14.221 | 1.00 | 0.00 |
| ATOM | 798 | CB | ASP | 1 | 507 | 33.592 | 37.776 | 14.228 | 1.00 | 0.00 |
| ATOM | 799 | CG | ASP | 1 | 507 | 33.701 | 38.921 | 13.260 | 1.00 | 0.00 |
| ATOM | 800 | OD1 | ASP | 1 | 507 | 34.544 | 39.786 | 13.435 | 1.00 | 0.00 |
| ATOM | 801 | OD2 | ASP | 1 | 507 | 32.884 | 38.995 | 12.355 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 802 | H | ASP | 1 | 507 | 33.406 | 35.688 | 15.357 | 1.00 | 0.00 |
| ATOM | 803 | N | ASN | 1 | 508 | 35.905 | 38.287 | 15.846 | 1.00 | 0.00 |
| ATOM | 804 | CA | ASN | 1 | 508 | 36.941 | 38.950 | 16.636 | 1.00 | 0.00 |
| ATOM | 805 | C | ASN | 1 | 508 | 37.554 | 40.207 | 16.003 | 1.00 | 0.00 |
| ATOM | 806 | O | ASN | 1 | 508 | 37.442 | 40.490 | 14.816 | 1.00 | 0.00 |
| ATOM | 807 | CB | ASN | 1 | 508 | 37.942 | 37.894 | 17.148 | 1.00 | 0.00 |
| ATOM | 808 | CG | ASN | 1 | 508 | 38.984 | 38.483 | 18.067 | 1.00 | 0.00 |
| ATOM | 809 | OD1 | ASN | 1 | 508 | 40.075 | 38.841 | 17.629 | 1.00 | 0.00 |
| ATOM | 810 | ND2 | ASN | 1 | 508 | 38.612 | 38.587 | 19.342 | 1.00 | 0.00 |
| ATOM | 811 | H | ASN | 1 | 508 | 34.972 | 38.528 | 16.098 | 1.00 | 0.00 |
| ATOM | 812 | 1HD2 | ASN | 1 | 508 | 39.255 | 38.836 | 20.065 | 1.00 | 0.00 |
| ATOM | 813 | 2HD2 | ASN | 1 | 508 | 37.657 | 38.470 | 19.612 | 1.00 | 0.00 |
| ATOM | 814 | N | LYS | 1 | 509 | 38.203 | 40.966 | 16.887 | 1.00 | 0.00 |
| ATOM | 815 | CA | LYS | 1 | 509 | 38.920 | 42.208 | 16.647 | 1.00 | 0.00 |
| ATOM | 816 | C | LYS | 1 | 509 | 38.126 | 43.497 | 16.680 | 1.00 | 0.00 |
| ATOM | 817 | O | LYS | 1 | 509 | 38.149 | 44.300 | 15.757 | 1.00 | 0.00 |
| ATOM | 818 | CB | LYS | 1 | 509 | 39.976 | 42.133 | 15.532 | 1.00 | 0.00 |
| ATOM | 819 | CG | LYS | 1 | 509 | 41.200 | 42.968 | 15.927 | 1.00 | 0.00 |
| ATOM | 820 | CD | LYS | 1 | 509 | 41.698 | 42.604 | 17.332 | 1.00 | 0.00 |
| ATOM | 821 | CE | LYS | 1 | 509 | 41.887 | 43.844 | 18.206 | 1.00 | 0.00 |
| ATOM | 822 | NZ | LYS | 1 | 509 | 41.436 | 43.564 | 19.565 | 1.00 | 0.00 |
| ATOM | 823 | H | LYS | 1 | 509 | 38.111 | 40.738 | 17.856 | 1.00 | 0.00 |
| ATOM | 824 | 1HZ | LYS | 1 | 509 | 42.164 | 43.009 | 20.053 | 1.00 | 0.00 |
| ATOM | 825 | 2HZ | LYS | 1 | 509 | 41.337 | 44.473 | 20.050 | 1.00 | 0.00 |
| ATOM | 826 | 3HZ | LYS | 1 | 509 | 40.546 | 43.027 | 19.604 | 1.00 | 0.00 |
| ATOM | 827 | N | ALA | 1 | 510 | 37.496 | 43.688 | 17.844 | 1.00 | 0.00 |
| ATOM | 828 | CA | ALA | 1 | 510 | 36.833 | 44.929 | 18.247 | 1.00 | 0.00 |
| ATOM | 829 | C | ALA | 1 | 510 | 37.482 | 46.239 | 17.852 | 1.00 | 0.00 |
| ATOM | 830 | O | ALA | 1 | 510 | 36.809 | 47.226 | 17.588 | 1.00 | 0.00 |
| ATOM | 831 | CB | ALA | 1 | 510 | 36.605 | 44.978 | 19.756 | 1.00 | 0.00 |
| ATOM | 832 | H | ALA | 1 | 510 | 37.421 | 42.899 | 18.451 | 1.00 | 0.00 |
| ATOM | 833 | N | ASP | 1 | 511 | 38.811 | 46.233 | 17.760 | 1.00 | 0.00 |
| ATOM | 834 | CA | ASP | 1 | 511 | 39.507 | 47.459 | 17.365 | 1.00 | 0.00 |
| ATOM | 835 | C | ASP | 1 | 511 | 39.701 | 47.501 | 15.852 | 1.00 | 0.00 |
| ATOM | 836 | O | ASP | 1 | 511 | 39.758 | 46.430 | 15.256 | 1.00 | 0.00 |
| ATOM | 837 | CB | ASP | 1 | 511 | 40.784 | 47.535 | 18.213 | 1.00 | 0.00 |
| ATOM | 838 | CG | ASP | 1 | 511 | 40.400 | 47.266 | 19.666 | 1.00 | 0.00 |
| ATOM | 839 | OD1 | ASP | 1 | 511 | 39.730 | 48.080 | 20.276 | 1.00 | 0.00 |
| ATOM | 840 | OD2 | ASP | 1 | 511 | 40.713 | 46.204 | 20.184 | 1.00 | 0.00 |
| ATOM | 841 | H | ASP | 1 | 511 | 39.298 | 45.425 | 18.087 | 1.00 | 0.00 |
| ATOM | 842 | N | LEU | 1 | 512 | 39.706 | 48.690 | 15.207 | 1.00 | 0.00 |
| ATOM | 843 | CA | LEU | 1 | 512 | 39.852 | 50.003 | 15.835 | 1.00 | 0.00 |
| ATOM | 844 | C | LEU | 1 | 512 | 38.524 | 50.631 | 16.191 | 1.00 | 0.00 |
| ATOM | 845 | O | LEU | 1 | 512 | 37.887 | 51.247 | 15.325 | 1.00 | 0.00 |
| ATOM | 846 | CB | LEU | 1 | 512 | 40.587 | 50.903 | 14.846 | 1.00 | 0.00 |
| ATOM | 847 | CG | LEU | 1 | 512 | 41.623 | 51.837 | 15.453 | 1.00 | 0.00 |
| ATOM | 848 | CD1 | LEU | 1 | 512 | 42.709 | 51.060 | 16.170 | 1.00 | 0.00 |
| ATOM | 849 | CD2 | LEU | 1 | 512 | 42.250 | 52.748 | 14.407 | 1.00 | 0.00 |
| ATOM | 850 | H | LEU | 1 | 512 | 39.438 | 48.632 | 14.248 | 1.00 | 0.00 |
| ATOM | 851 | N | ALA | 1 | 513 | 38.142 | 50.407 | 17.443 | 1.00 | 0.00 |
| ATOM | 852 | CA | ALA | 1 | 513 | 36.827 | 50.802 | 17.922 | 1.00 | 0.00 |
| ATOM | 853 | C | ALA | 1 | 513 | 36.726 | 52.265 | 18.267 | 1.00 | 0.00 |
| ATOM | 854 | O | ALA | 1 | 513 | 37.592 | 52.788 | 18.966 | 1.00 | 0.00 |
| ATOM | 855 | CB | ALA | 1 | 513 | 36.538 | 50.043 | 19.219 | 1.00 | 0.00 |
| ATOM | 856 | H | ALA | 1 | 513 | 38.778 | 49.963 | 18.071 | 1.00 | 0.00 |
| ATOM | 857 | N | VAL | 1 | 514 | 35.619 | 52.913 | 17.879 | 1.00 | 0.00 |
| ATOM | 858 | CA | VAL | 1 | 514 | 35.372 | 54.140 | 18.634 | 1.00 | 0.00 |
| ATOM | 859 | C | VAL | 1 | 514 | 34.445 | 53.965 | 19.835 | 1.00 | 0.00 |
| ATOM | 860 | O | VAL | 1 | 514 | 34.855 | 53.346 | 20.814 | 1.00 | 0.00 |
| ATOM | 861 | CB | VAL | 1 | 514 | 35.045 | 55.351 | 17.756 | 1.00 | 0.00 |
| ATOM | 862 | CG1 | VAL | 1 | 514 | 35.399 | 56.636 | 18.515 | 1.00 | 0.00 |
| ATOM | 863 | CG2 | VAL | 1 | 514 | 35.800 | 55.303 | 16.428 | 1.00 | 0.00 |
| ATOM | 864 | H | VAL | 1 | 514 | 35.025 | 52.532 | 17.168 | 1.00 | 0.00 |
| ATOM | 865 | N | ALA | 1 | 515 | 33.211 | 54.521 | 19.793 | 1.00 | 0.00 |
| ATOM | 866 | CA | ALA | 1 | 515 | 32.345 | 54.521 | 20.991 | 1.00 | 0.00 |
| ATOM | 867 | C | ALA | 1 | 515 | 33.015 | 54.962 | 22.284 | 1.00 | 0.00 |
| ATOM | 868 | O | ALA | 1 | 515 | 33.467 | 54.141 | 23.089 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 869 | CB | ALA | 1 | 515 | 31.749 | 53.148 | 21.254 | 1.00 | 0.00 |
| ATOM | 870 | H | ALA | 1 | 515 | 32.845 | 54.928 | 18.954 | 1.00 | 0.00 |
| ATOM | 871 | N | PRO | 1 | 516 | 33.115 | 56.302 | 22.424 | 1.00 | 0.00 |
| ATOM | 872 | CA | PRO | 1 | 516 | 34.051 | 56.917 | 23.374 | 1.00 | 0.00 |
| ATOM | 873 | C | PRO | 1 | 516 | 34.288 | 56.241 | 24.720 | 1.00 | 0.00 |
| ATOM | 874 | O | PRO | 1 | 516 | 33.543 | 56.474 | 25.680 | 1.00 | 0.00 |
| ATOM | 875 | CB | PRO | 1 | 516 | 33.528 | 58.351 | 23.444 | 1.00 | 0.00 |
| ATOM | 876 | CG | PRO | 1 | 516 | 32.978 | 58.626 | 22.045 | 1.00 | 0.00 |
| ATOM | 877 | CD | PRO | 1 | 516 | 32.368 | 57.289 | 21.649 | 1.00 | 0.00 |
| ATOM | 878 | N | LEU | 1 | 517 | 35.386 | 55.429 | 24.674 | 1.00 | 0.00 |
| ATOM | 879 | CA | LEU | 1 | 517 | 35.982 | 54.630 | 25.757 | 1.00 | 0.00 |
| ATOM | 880 | C | LEU | 1 | 517 | 36.180 | 55.353 | 27.080 | 1.00 | 0.00 |
| ATOM | 881 | O | LEU | 1 | 517 | 35.242 | 56.016 | 27.513 | 1.00 | 0.00 |
| ATOM | 882 | CB | LEU | 1 | 517 | 37.285 | 53.964 | 25.296 | 1.00 | 0.00 |
| ATOM | 883 | CG | LEU | 1 | 517 | 37.266 | 53.197 | 23.975 | 1.00 | 0.00 |
| ATOM | 884 | CD1 | LEU | 1 | 517 | 38.648 | 52.612 | 23.717 | 1.00 | 0.00 |
| ATOM | 885 | CD2 | LEU | 1 | 517 | 36.172 | 52.134 | 23.872 | 1.00 | 0.00 |
| ATOM | 886 | H | LEU | 1 | 517 | 35.840 | 55.344 | 23.790 | 1.00 | 0.00 |
| ATOM | 887 | N | ALA | 1 | 518 | 37.339 | 55.204 | 27.760 | 1.00 | 0.00 |
| ATOM | 888 | CA | ALA | 1 | 518 | 37.367 | 55.922 | 29.035 | 1.00 | 0.00 |
| ATOM | 889 | C | ALA | 1 | 518 | 38.692 | 56.480 | 29.490 | 1.00 | 0.00 |
| ATOM | 890 | O | ALA | 1 | 518 | 39.675 | 55.759 | 29.661 | 1.00 | 0.00 |
| ATOM | 891 | CB | ALA | 1 | 518 | 36.790 | 55.097 | 30.188 | 1.00 | 0.00 |
| ATOM | 892 | H | ALA | 1 | 518 | 38.165 | 54.773 | 27.410 | 1.00 | 0.00 |
| ATOM | 893 | N | ILE | 1 | 519 | 38.679 | 57.804 | 29.738 | 1.00 | 0.00 |
| ATOM | 894 | CA | ILE | 1 | 519 | 39.860 | 58.449 | 30.319 | 1.00 | 0.00 |
| ATOM | 895 | C | ILE | 1 | 519 | 40.006 | 58.165 | 31.815 | 1.00 | 0.00 |
| ATOM | 896 | O | ILE | 1 | 519 | 39.660 | 58.921 | 32.728 | 1.00 | 0.00 |
| ATOM | 897 | CB | ILE | 1 | 519 | 39.900 | 59.943 | 29.930 | 1.00 | 0.00 |
| ATOM | 898 | CG1 | ILE | 1 | 519 | 41.158 | 60.648 | 30.449 | 1.00 | 0.00 |
| ATOM | 899 | CG2 | ILE | 1 | 519 | 38.623 | 60.683 | 30.350 | 1.00 | 0.00 |
| ATOM | 900 | CD1 | ILE | 1 | 519 | 41.291 | 62.087 | 29.949 | 1.00 | 0.00 |
| ATOM | 901 | H | ILE | 1 | 519 | 37.799 | 58.275 | 29.674 | 1.00 | 0.00 |
| ATOM | 902 | N | THR | 1 | 520 | 40.493 | 56.941 | 32.021 | 1.00 | 0.00 |
| ATOM | 903 | CA | THR | 1 | 520 | 40.527 | 56.340 | 33.352 | 1.00 | 0.00 |
| ATOM | 904 | C | THR | 1 | 520 | 41.418 | 55.132 | 33.262 | 1.00 | 0.00 |
| ATOM | 905 | O | THR | 1 | 520 | 41.121 | 54.204 | 32.516 | 1.00 | 0.00 |
| ATOM | 906 | CB | THR | 1 | 520 | 39.135 | 55.888 | 33.836 | 1.00 | 0.00 |
| ATOM | 907 | OG1 | THR | 1 | 520 | 38.158 | 56.932 | 33.707 | 1.00 | 0.00 |
| ATOM | 908 | CG2 | THR | 1 | 520 | 39.170 | 55.412 | 35.290 | 1.00 | 0.00 |
| ATOM | 909 | H | THR | 1 | 520 | 40.827 | 56.428 | 31.227 | 1.00 | 0.00 |
| ATOM | 910 | HG1 | THR | 1 | 520 | 38.218 | 57.221 | 32.798 | 1.00 | 0.00 |
| ATOM | 911 | N | TYR | 1 | 521 | 42.510 | 55.194 | 34.034 | 1.00 | 0.00 |
| ATOM | 912 | CA | TYR | 1 | 521 | 43.519 | 54.136 | 34.011 | 1.00 | 0.00 |
| ATOM | 913 | C | TYR | 1 | 521 | 42.972 | 52.717 | 34.022 | 1.00 | 0.00 |
| ATOM | 914 | O | TYR | 1 | 521 | 43.315 | 51.876 | 33.204 | 1.00 | 0.00 |
| ATOM | 915 | CB | TYR | 1 | 521 | 44.529 | 54.365 | 35.142 | 1.00 | 0.00 |
| ATOM | 916 | CG | TYR | 1 | 521 | 45.811 | 53.606 | 34.883 | 1.00 | 0.00 |
| ATOM | 917 | CD1 | TYR | 1 | 521 | 46.078 | 52.440 | 35.628 | 1.00 | 0.00 |
| ATOM | 918 | CD2 | TYR | 1 | 521 | 46.707 | 54.088 | 33.906 | 1.00 | 0.00 |
| ATOM | 919 | CE1 | TYR | 1 | 521 | 47.276 | 51.744 | 35.397 | 1.00 | 0.00 |
| ATOM | 920 | CE2 | TYR | 1 | 521 | 47.900 | 53.388 | 33.668 | 1.00 | 0.00 |
| ATOM | 921 | CZ | TYR | 1 | 521 | 48.172 | 52.229 | 34.422 | 1.00 | 0.00 |
| ATOM | 922 | OH | TYR | 1 | 521 | 49.355 | 51.548 | 34.204 | 1.00 | 0.00 |
| ATOM | 923 | H | TYR | 1 | 521 | 42.666 | 56.063 | 34.498 | 1.00 | 0.00 |
| ATOM | 924 | HH | TYR | 1 | 521 | 49.680 | 51.260 | 35.053 | 1.00 | 0.00 |
| ATOM | 925 | N | VAL | 1 | 522 | 42.044 | 52.495 | 34.967 | 1.00 | 0.00 |
| ATOM | 926 | CA | VAL | 1 | 522 | 41.474 | 51.148 | 35.058 | 1.00 | 0.00 |
| ATOM | 927 | C | VAL | 1 | 522 | 40.750 | 50.610 | 33.825 | 1.00 | 0.00 |
| ATOM | 928 | O | VAL | 1 | 522 | 40.532 | 49.411 | 33.710 | 1.00 | 0.00 |
| ATOM | 929 | CB | VAL | 1 | 522 | 40.609 | 50.988 | 36.318 | 1.00 | 0.00 |
| ATOM | 930 | CG1 | VAL | 1 | 522 | 41.435 | 51.280 | 37.573 | 1.00 | 0.00 |
| ATOM | 931 | CG2 | VAL | 1 | 522 | 39.321 | 51.814 | 36.264 | 1.00 | 0.00 |
| ATOM | 932 | H | VAL | 1 | 522 | 41.749 | 53.248 | 35.551 | 1.00 | 0.00 |
| ATOM | 933 | N | ARG | 1 | 523 | 40.407 | 51.525 | 32.903 | 1.00 | 0.00 |
| ATOM | 934 | CA | ARG | 1 | 523 | 39.845 | 51.140 | 31.601 | 1.00 | 0.00 |
| ATOM | 935 | C | ARG | 1 | 523 | 40.841 | 51.230 | 30.448 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 936 | O | ARG | 1 | 523 | 40.931 | 50.357 | 29.588 | 1.00 | 0.00 |
| ATOM | 937 | CB | ARG | 1 | 523 | 38.639 | 52.033 | 31.310 | 1.00 | 0.00 |
| ATOM | 938 | CG | ARG | 1 | 523 | 38.104 | 51.998 | 29.873 | 1.00 | 0.00 |
| ATOM | 939 | CD | ARG | 1 | 523 | 37.275 | 50.777 | 29.514 | 1.00 | 0.00 |
| ATOM | 940 | NE | ARG | 1 | 523 | 36.691 | 50.922 | 28.179 | 1.00 | 0.00 |
| ATOM | 941 | CZ | ARG | 1 | 523 | 35.413 | 51.324 | 27.987 | 1.00 | 0.00 |
| ATOM | 942 | NH1 | ARG | 1 | 523 | 34.864 | 51.131 | 26.797 | 1.00 | 0.00 |
| ATOM | 943 | NH2 | ARG | 1 | 523 | 34.701 | 51.896 | 28.957 | 1.00 | 0.00 |
| ATOM | 944 | H | ARG | 1 | 523 | 40.625 | 52.479 | 33.105 | 1.00 | 0.00 |
| ATOM | 945 | HE | ARG | 1 | 523 | 37.217 | 50.624 | 27.372 | 1.00 | 0.00 |
| ATOM | 946 | 1HH1 | ARG | 1 | 523 | 33.895 | 51.340 | 26.672 | 1.00 | 0.00 |
| ATOM | 947 | 2HH1 | ARG | 1 | 523 | 35.395 | 50.754 | 26.024 | 1.00 | 0.00 |
| ATOM | 948 | 1HH2 | ARG | 1 | 523 | 33.735 | 52.119 | 28.818 | 1.00 | 0.00 |
| ATOM | 949 | 2HH2 | ARG | 1 | 523 | 35.122 | 52.139 | 29.832 | 1.00 | 0.00 |
| ATOM | 950 | N | GLU | 1 | 524 | 41.578 | 52.346 | 30.452 | 1.00 | 0.00 |
| ATOM | 951 | CA | GLU | 1 | 524 | 42.519 | 52.620 | 29.376 | 1.00 | 0.00 |
| ATOM | 952 | C | GLU | 1 | 524 | 43.662 | 51.627 | 29.354 | 1.00 | 0.00 |
| ATOM | 953 | O | GLU | 1 | 524 | 44.114 | 51.170 | 28.304 | 1.00 | 0.00 |
| ATOM | 954 | CB | GLU | 1 | 524 | 42.926 | 54.096 | 29.474 | 1.00 | 0.00 |
| ATOM | 955 | CG | GLU | 1 | 524 | 44.347 | 54.501 | 29.057 | 1.00 | 0.00 |
| ATOM | 956 | CD | GLU | 1 | 524 | 45.367 | 54.129 | 30.118 | 1.00 | 0.00 |
| ATOM | 957 | OE1 | GLU | 1 | 524 | 44.997 | 53.899 | 31.263 | 1.00 | 0.00 |
| ATOM | 958 | OE2 | GLU | 1 | 524 | 46.546 | 54.059 | 29.801 | 1.00 | 0.00 |
| ATOM | 959 | H | GLU | 1 | 524 | 41.509 | 53.004 | 31.195 | 1.00 | 0.00 |
| ATOM | 960 | N | LYS | 1 | 525 | 44.065 | 51.224 | 30.568 | 1.00 | 0.00 |
| ATOM | 961 | CA | LYS | 1 | 525 | 45.011 | 50.119 | 30.602 | 1.00 | 0.00 |
| ATOM | 962 | C | LYS | 1 | 525 | 44.415 | 48.724 | 30.650 | 1.00 | 0.00 |
| ATOM | 963 | O | LYS | 1 | 525 | 45.097 | 47.724 | 30.858 | 1.00 | 0.00 |
| ATOM | 964 | CB | LYS | 1 | 525 | 46.086 | 50.355 | 31.659 | 1.00 | 0.00 |
| ATOM | 965 | CG | LYS | 1 | 525 | 47.519 | 50.222 | 31.121 | 1.00 | 0.00 |
| ATOM | 966 | CD | LYS | 1 | 525 | 47.961 | 51.280 | 30.093 | 1.00 | 0.00 |
| ATOM | 967 | CE | LYS | 1 | 525 | 47.645 | 50.993 | 28.616 | 1.00 | 0.00 |
| ATOM | 968 | NZ | LYS | 1 | 525 | 46.705 | 51.957 | 28.016 | 1.00 | 0.00 |
| ATOM | 969 | H | LYS | 1 | 525 | 43.748 | 51.666 | 31.405 | 1.00 | 0.00 |
| ATOM | 970 | 1HZ | LYS | 1 | 525 | 46.669 | 52.862 | 28.525 | 1.00 | 0.00 |
| ATOM | 971 | 2HZ | LYS | 1 | 525 | 47.019 | 52.159 | 27.045 | 1.00 | 0.00 |
| ATOM | 972 | 3HZ | LYS | 1 | 525 | 45.743 | 51.571 | 27.912 | 1.00 | 0.00 |
| ATOM | 973 | N | VAL | 1 | 526 | 43.103 | 48.686 | 30.369 | 1.00 | 0.00 |
| ATOM | 974 | CA | VAL | 1 | 526 | 42.623 | 47.462 | 29.738 | 1.00 | 0.00 |
| ATOM | 975 | C | VAL | 1 | 526 | 42.767 | 47.608 | 28.233 | 1.00 | 0.00 |
| ATOM | 976 | O | VAL | 1 | 526 | 43.608 | 46.962 | 27.614 | 1.00 | 0.00 |
| ATOM | 977 | CB | VAL | 1 | 526 | 41.181 | 47.124 | 30.153 | 1.00 | 0.00 |
| ATOM | 978 | CG1 | VAL | 1 | 526 | 40.667 | 45.843 | 29.485 | 1.00 | 0.00 |
| ATOM | 979 | CG2 | VAL | 1 | 526 | 41.078 | 47.018 | 31.674 | 1.00 | 0.00 |
| ATOM | 980 | H | VAL | 1 | 526 | 42.552 | 49.511 | 30.284 | 1.00 | 0.00 |
| ATOM | 981 | N | ILE | 1 | 527 | 41.943 | 48.508 | 27.675 | 1.00 | 0.00 |
| ATOM | 982 | CA | ILE | 1 | 527 | 42.036 | 48.762 | 26.236 | 1.00 | 0.00 |
| ATOM | 983 | C | ILE | 1 | 527 | 42.563 | 50.147 | 25.910 | 1.00 | 0.00 |
| ATOM | 984 | O | ILE | 1 | 527 | 42.088 | 51.164 | 26.426 | 1.00 | 0.00 |
| ATOM | 985 | CB | ILE | 1 | 527 | 40.701 | 48.489 | 25.523 | 1.00 | 0.00 |
| ATOM | 986 | CG1 | ILE | 1 | 527 | 39.528 | 49.266 | 26.133 | 1.00 | 0.00 |
| ATOM | 987 | CG2 | ILE | 1 | 527 | 40.421 | 46.983 | 25.529 | 1.00 | 0.00 |
| ATOM | 988 | CD1 | ILE | 1 | 527 | 38.219 | 49.052 | 25.370 | 1.00 | 0.00 |
| ATOM | 989 | H | ILE | 1 | 527 | 41.358 | 49.022 | 28.299 | 1.00 | 0.00 |
| ATOM | 990 | N | ASP | 1 | 528 | 43.593 | 50.135 | 25.050 | 1.00 | 0.00 |
| ATOM | 991 | CA | ASP | 1 | 528 | 44.293 | 51.389 | 24.761 | 1.00 | 0.00 |
| ATOM | 992 | C | ASP | 1 | 528 | 43.502 | 52.440 | 24.014 | 1.00 | 0.00 |
| ATOM | 993 | O | ASP | 1 | 528 | 42.364 | 52.206 | 23.626 | 1.00 | 0.00 |
| ATOM | 994 | CB | ASP | 1 | 528 | 45.619 | 51.118 | 24.083 | 1.00 | 0.00 |
| ATOM | 995 | CG | ASP | 1 | 528 | 46.679 | 51.004 | 25.138 | 1.00 | 0.00 |
| ATOM | 996 | OD1 | ASP | 1 | 528 | 47.396 | 51.971 | 25.331 | 1.00 | 0.00 |
| ATOM | 997 | OD2 | ASP | 1 | 528 | 46.782 | 49.975 | 25.793 | 1.00 | 0.00 |
| ATOM | 998 | H | ASP | 1 | 528 | 43.912 | 49.263 | 24.675 | 1.00 | 0.00 |
| ATOM | 999 | N | PHE | 1 | 529 | 44.096 | 53.635 | 23.925 | 1.00 | 0.00 |
| ATOM | 1000 | CA | PHE | 1 | 529 | 43.208 | 54.794 | 23.919 | 1.00 | 0.00 |
| ATOM | 1001 | C | PHE | 1 | 529 | 43.396 | 55.695 | 22.718 | 1.00 | 0.00 |
| ATOM | 1002 | O | PHE | 1 | 529 | 44.401 | 55.608 | 22.033 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1003 | CB | PHE | 1 | 529 | 43.422 | 55.553 | 25.234 | 1.00 | 0.00 |
| ATOM | 1004 | CG | PHE | 1 | 529 | 44.839 | 56.073 | 25.389 | 1.00 | 0.00 |
| ATOM | 1005 | CD1 | PHE | 1 | 529 | 45.136 | 57.396 | 24.993 | 1.00 | 0.00 |
| ATOM | 1006 | CD2 | PHE | 1 | 529 | 45.841 | 55.238 | 25.933 | 1.00 | 0.00 |
| ATOM | 1007 | CE1 | PHE | 1 | 529 | 46.446 | 57.890 | 25.138 | 1.00 | 0.00 |
| ATOM | 1008 | CE2 | PHE | 1 | 529 | 47.152 | 55.727 | 26.080 | 1.00 | 0.00 |
| ATOM | 1009 | CZ | PHE | 1 | 529 | 47.441 | 57.049 | 25.680 | 1.00 | 0.00 |
| ATOM | 1010 | H | PHE | 1 | 529 | 45.084 | 53.752 | 24.023 | 1.00 | 0.00 |
| ATOM | 1011 | N | SER | 1 | 530 | 42.449 | 56.610 | 22.491 | 1.00 | 0.00 |
| ATOM | 1012 | CA | SER | 1 | 530 | 42.784 | 57.761 | 21.641 | 1.00 | 0.00 |
| ATOM | 1013 | C | SER | 1 | 530 | 43.103 | 58.885 | 22.593 | 1.00 | 0.00 |
| ATOM | 1014 | O | SER | 1 | 530 | 42.601 | 58.853 | 23.715 | 1.00 | 0.00 |
| ATOM | 1015 | CB | SER | 1 | 530 | 41.578 | 58.152 | 20.779 | 1.00 | 0.00 |
| ATOM | 1016 | OG | SER | 1 | 530 | 41.862 | 59.210 | 19.849 | 1.00 | 0.00 |
| ATOM | 1017 | H | SER | 1 | 530 | 41.682 | 56.626 | 23.125 | 1.00 | 0.00 |
| ATOM | 1018 | HG | SER | 1 | 530 | 42.572 | 58.900 | 19.281 | 1.00 | 0.00 |
| ATOM | 1019 | N | LYS | 1 | 531 | 43.906 | 59.849 | 22.145 | 1.00 | 0.00 |
| ATOM | 1020 | CA | LYS | 1 | 531 | 44.011 | 61.088 | 22.924 | 1.00 | 0.00 |
| ATOM | 1021 | C | LYS | 1 | 531 | 42.700 | 61.868 | 22.786 | 1.00 | 0.00 |
| ATOM | 1022 | O | LYS | 1 | 531 | 42.095 | 61.787 | 21.717 | 1.00 | 0.00 |
| ATOM | 1023 | CB | LYS | 1 | 531 | 45.239 | 61.854 | 22.416 | 1.00 | 0.00 |
| ATOM | 1024 | CG | LYS | 1 | 531 | 45.803 | 62.837 | 23.438 | 1.00 | 0.00 |
| ATOM | 1025 | CD | LYS | 1 | 531 | 46.367 | 62.166 | 24.693 | 1.00 | 0.00 |
| ATOM | 1026 | CE | LYS | 1 | 531 | 46.280 | 63.048 | 25.946 | 1.00 | 0.00 |
| ATOM | 1027 | NZ | LYS | 1 | 531 | 46.653 | 64.430 | 25.652 | 1.00 | 0.00 |
| ATOM | 1028 | H | LYS | 1 | 531 | 44.227 | 59.745 | 21.205 | 1.00 | 0.00 |
| ATOM | 1029 | 1HZ | LYS | 1 | 531 | 47.043 | 64.875 | 26.490 | 1.00 | 0.00 |
| ATOM | 1030 | 2HZ | LYS | 1 | 531 | 47.400 | 64.466 | 24.933 | 1.00 | 0.00 |
| ATOM | 1031 | 3HZ | LYS | 1 | 531 | 45.840 | 65.026 | 25.382 | 1.00 | 0.00 |
| ATOM | 1032 | N | PRO | 1 | 532 | 42.209 | 62.519 | 23.883 | 1.00 | 0.00 |
| ATOM | 1033 | CA | PRO | 1 | 532 | 40.922 | 63.232 | 23.893 | 1.00 | 0.00 |
| ATOM | 1034 | C | PRO | 1 | 532 | 40.530 | 64.180 | 22.772 | 1.00 | 0.00 |
| ATOM | 1035 | O | PRO | 1 | 532 | 40.362 | 65.386 | 22.930 | 1.00 | 0.00 |
| ATOM | 1036 | CB | PRO | 1 | 532 | 40.881 | 63.894 | 25.272 | 1.00 | 0.00 |
| ATOM | 1037 | CG | PRO | 1 | 532 | 41.659 | 62.932 | 26.155 | 1.00 | 0.00 |
| ATOM | 1038 | CD | PRO | 1 | 532 | 42.775 | 62.481 | 25.225 | 1.00 | 0.00 |
| ATOM | 1039 | N | PHE | 1 | 533 | 40.224 | 63.550 | 21.639 | 1.00 | 0.00 |
| ATOM | 1040 | CA | PHE | 1 | 533 | 39.367 | 64.248 | 20.694 | 1.00 | 0.00 |
| ATOM | 1041 | C | PHE | 1 | 533 | 37.905 | 63.950 | 20.975 | 1.00 | 0.00 |
| ATOM | 1042 | O | PHE | 1 | 533 | 36.999 | 64.214 | 20.179 | 1.00 | 0.00 |
| ATOM | 1043 | CB | PHE | 1 | 533 | 39.748 | 63.884 | 19.257 | 1.00 | 0.00 |
| ATOM | 1044 | CG | PHE | 1 | 533 | 41.087 | 64.492 | 18.904 | 1.00 | 0.00 |
| ATOM | 1045 | CD1 | PHE | 1 | 533 | 41.122 | 65.695 | 18.166 | 1.00 | 0.00 |
| ATOM | 1046 | CD2 | PHE | 1 | 533 | 42.280 | 63.856 | 19.317 | 1.00 | 0.00 |
| ATOM | 1047 | CE1 | PHE | 1 | 533 | 42.363 | 66.276 | 17.846 | 1.00 | 0.00 |
| ATOM | 1048 | CE2 | PHE | 1 | 533 | 43.522 | 64.435 | 19.000 | 1.00 | 0.00 |
| ATOM | 1049 | CZ | PHE | 1 | 533 | 43.549 | 65.640 | 18.270 | 1.00 | 0.00 |
| ATOM | 1050 | H | PHE | 1 | 533 | 40.363 | 62.563 | 21.573 | 1.00 | 0.00 |
| ATOM | 1051 | N | MET | 1 | 534 | 37.663 | 63.363 | 22.163 | 1.00 | 0.00 |
| ATOM | 1052 | CA | MET | 1 | 534 | 36.268 | 63.187 | 22.534 | 1.00 | 0.00 |
| ATOM | 1053 | C | MET | 1 | 534 | 35.792 | 64.164 | 23.582 | 1.00 | 0.00 |
| ATOM | 1054 | O | MET | 1 | 534 | 34.653 | 64.613 | 23.509 | 1.00 | 0.00 |
| ATOM | 1055 | CB | MET | 1 | 534 | 35.965 | 61.747 | 22.958 | 1.00 | 0.00 |
| ATOM | 1056 | CG | MET | 1 | 534 | 36.155 | 60.730 | 21.830 | 1.00 | 0.00 |
| ATOM | 1057 | SD | MET | 1 | 534 | 37.867 | 60.539 | 21.309 | 1.00 | 0.00 |
| ATOM | 1058 | CE | MET | 1 | 534 | 37.566 | 59.773 | 19.713 | 1.00 | 0.00 |
| ATOM | 1059 | H | MET | 1 | 534 | 38.424 | 63.128 | 22.766 | 1.00 | 0.00 |
| ATOM | 1060 | N | THR | 1 | 535 | 36.692 | 64.448 | 24.544 | 1.00 | 0.00 |
| ATOM | 1061 | CA | THR | 1 | 535 | 36.344 | 64.966 | 25.871 | 1.00 | 0.00 |
| ATOM | 1062 | C | THR | 1 | 535 | 34.979 | 65.610 | 26.079 | 1.00 | 0.00 |
| ATOM | 1063 | O | THR | 1 | 535 | 34.688 | 66.738 | 25.667 | 1.00 | 0.00 |
| ATOM | 1064 | CB | THR | 1 | 535 | 37.518 | 65.795 | 26.443 | 1.00 | 0.00 |
| ATOM | 1065 | OG1 | THR | 1 | 535 | 37.350 | 66.086 | 27.844 | 1.00 | 0.00 |
| ATOM | 1066 | CG2 | THR | 1 | 535 | 37.814 | 67.063 | 25.635 | 1.00 | 0.00 |
| ATOM | 1067 | H | THR | 1 | 535 | 37.624 | 64.123 | 24.427 | 1.00 | 0.00 |
| ATOM | 1068 | HG1 | THR | 1 | 535 | 38.166 | 66.524 | 28.096 | 1.00 | 0.00 |
| ATOM | 1069 | N | LEU | 1 | 536 | 34.135 | 64.832 | 26.749 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1070 | CA | LEU | 1 | 536 | 32.983 | 65.429 | 27.401 | 1.00 | 0.00 |
| ATOM | 1071 | C | LEU | 1 | 536 | 33.266 | 65.466 | 28.879 | 1.00 | 0.00 |
| ATOM | 1072 | O | LEU | 1 | 536 | 34.006 | 64.639 | 29.409 | 1.00 | 0.00 |
| ATOM | 1073 | CB | LEU | 1 | 536 | 31.690 | 64.641 | 27.156 | 1.00 | 0.00 |
| ATOM | 1074 | CG | LEU | 1 | 536 | 31.091 | 64.783 | 25.752 | 1.00 | 0.00 |
| ATOM | 1075 | CD1 | LEU | 1 | 536 | 31.083 | 66.241 | 25.288 | 1.00 | 0.00 |
| ATOM | 1076 | CD2 | LEU | 1 | 536 | 31.724 | 63.836 | 24.732 | 1.00 | 0.00 |
| ATOM | 1077 | H | LEU | 1 | 536 | 34.394 | 63.899 | 26.978 | 1.00 | 0.00 |
| ATOM | 1078 | N | GLY | 1 | 537 | 32.658 | 66.449 | 29.522 | 1.00 | 0.00 |
| ATOM | 1079 | CA | GLY | 1 | 537 | 32.802 | 66.432 | 30.965 | 1.00 | 0.00 |
| ATOM | 1080 | C | GLY | 1 | 537 | 31.683 | 65.648 | 31.604 | 1.00 | 0.00 |
| ATOM | 1081 | O | GLY | 1 | 537 | 30.673 | 65.304 | 30.984 | 1.00 | 0.00 |
| ATOM | 1082 | H | GLY | 1 | 537 | 31.992 | 67.030 | 29.069 | 1.00 | 0.00 |
| ATOM | 1083 | N | ILE | 1 | 538 | 31.867 | 65.422 | 32.919 | 1.00 | 0.00 |
| ATOM | 1084 | CA | ILE | 1 | 538 | 30.642 | 65.108 | 33.643 | 1.00 | 0.00 |
| ATOM | 1085 | C | ILE | 1 | 538 | 29.951 | 66.406 | 33.941 | 1.00 | 0.00 |
| ATOM | 1086 | O | ILE | 1 | 538 | 30.570 | 67.452 | 34.173 | 1.00 | 0.00 |
| ATOM | 1087 | CB | ILE | 1 | 538 | 30.857 | 64.257 | 34.907 | 1.00 | 0.00 |
| ATOM | 1088 | CG1 | ILE | 1 | 538 | 29.616 | 63.426 | 35.235 | 1.00 | 0.00 |
| ATOM | 1089 | CG2 | ILE | 1 | 538 | 31.326 | 65.054 | 36.136 | 1.00 | 0.00 |
| ATOM | 1090 | CD1 | ILE | 1 | 538 | 29.906 | 62.330 | 36.260 | 1.00 | 0.00 |
| ATOM | 1091 | H | ILE | 1 | 538 | 32.650 | 65.836 | 33.382 | 1.00 | 0.00 |
| ATOM | 1092 | N | SER | 1 | 539 | 28.639 | 66.329 | 33.867 | 1.00 | 0.00 |
| ATOM | 1093 | CA | SER | 1 | 539 | 27.982 | 67.608 | 33.933 | 1.00 | 0.00 |
| ATOM | 1094 | C | SER | 1 | 539 | 26.999 | 67.638 | 35.069 | 1.00 | 0.00 |
| ATOM | 1095 | O | SER | 1 | 539 | 26.137 | 66.781 | 35.265 | 1.00 | 0.00 |
| ATOM | 1096 | CB | SER | 1 | 539 | 27.472 | 67.947 | 32.545 | 1.00 | 0.00 |
| ATOM | 1097 | OG | SER | 1 | 539 | 28.463 | 67.531 | 31.578 | 1.00 | 0.00 |
| ATOM | 1098 | H | SER | 1 | 539 | 28.189 | 65.471 | 33.617 | 1.00 | 0.00 |
| ATOM | 1099 | HG | SER | 1 | 539 | 28.566 | 66.589 | 31.779 | 1.00 | 0.00 |
| ATOM | 1100 | N | ILE | 1 | 540 | 27.304 | 68.614 | 35.907 | 1.00 | 0.00 |
| ATOM | 1101 | CA | ILE | 1 | 540 | 26.815 | 68.569 | 37.276 | 1.00 | 0.00 |
| ATOM | 1102 | C | ILE | 1 | 540 | 25.624 | 69.502 | 37.330 | 1.00 | 0.00 |
| ATOM | 1103 | O | ILE | 1 | 540 | 25.406 | 70.250 | 36.376 | 1.00 | 0.00 |
| ATOM | 1104 | CB | ILE | 1 | 540 | 28.004 | 68.957 | 38.188 | 1.00 | 0.00 |
| ATOM | 1105 | CG1 | ILE | 1 | 540 | 29.222 | 68.119 | 37.771 | 1.00 | 0.00 |
| ATOM | 1106 | CG2 | ILE | 1 | 540 | 27.736 | 68.727 | 39.682 | 1.00 | 0.00 |
| ATOM | 1107 | CD1 | ILE | 1 | 540 | 30.547 | 68.528 | 38.406 | 1.00 | 0.00 |
| ATOM | 1108 | H | ILE | 1 | 540 | 27.847 | 69.372 | 35.549 | 1.00 | 0.00 |
| ATOM | 1109 | N | LEU | 1 | 541 | 24.875 | 69.463 | 38.430 | 1.00 | 0.00 |
| ATOM | 1110 | CA | LEU | 1 | 541 | 23.722 | 70.350 | 38.589 | 1.00 | 0.00 |
| ATOM | 1111 | C | LEU | 1 | 541 | 22.748 | 70.274 | 37.438 | 1.00 | 0.00 |
| ATOM | 1112 | O | LEU | 1 | 541 | 22.285 | 71.263 | 36.872 | 1.00 | 0.00 |
| ATOM | 1113 | CB | LEU | 1 | 541 | 24.068 | 71.826 | 38.857 | 1.00 | 0.00 |
| ATOM | 1114 | CG | LEU | 1 | 541 | 25.111 | 72.146 | 39.931 | 1.00 | 0.00 |
| ATOM | 1115 | CD1 | LEU | 1 | 541 | 25.018 | 71.244 | 41.162 | 1.00 | 0.00 |
| ATOM | 1116 | CD2 | LEU | 1 | 541 | 26.516 | 72.212 | 39.344 | 1.00 | 0.00 |
| ATOM | 1117 | H | LEU | 1 | 541 | 25.073 | 68.726 | 39.067 | 1.00 | 0.00 |
| ATOM | 1118 | N | TYR | 1 | 542 | 22.420 | 69.020 | 37.110 | 1.00 | 0.00 |
| ATOM | 1119 | CA | TYR | 1 | 542 | 21.221 | 68.906 | 36.285 | 1.00 | 0.00 |
| ATOM | 1120 | C | TYR | 1 | 542 | 19.997 | 69.016 | 37.156 | 1.00 | 0.00 |
| ATOM | 1121 | O | TYR | 1 | 542 | 19.539 | 68.079 | 37.810 | 1.00 | 0.00 |
| ATOM | 1122 | CB | TYR | 1 | 542 | 21.269 | 67.694 | 35.341 | 1.00 | 0.00 |
| ATOM | 1123 | CG | TYR | 1 | 542 | 22.240 | 68.044 | 34.234 | 1.00 | 0.00 |
| ATOM | 1124 | CD1 | TYR | 1 | 542 | 21.761 | 68.217 | 32.921 | 1.00 | 0.00 |
| ATOM | 1125 | CD2 | TYR | 1 | 542 | 23.591 | 68.266 | 34.554 | 1.00 | 0.00 |
| ATOM | 1126 | CE1 | TYR | 1 | 542 | 22.608 | 68.782 | 31.951 | 1.00 | 0.00 |
| ATOM | 1127 | CE2 | TYR | 1 | 542 | 24.430 | 68.842 | 33.599 | 1.00 | 0.00 |
| ATOM | 1128 | CZ | TYR | 1 | 542 | 23.918 | 69.135 | 32.327 | 1.00 | 0.00 |
| ATOM | 1129 | OH | TYR | 1 | 542 | 24.731 | 69.808 | 31.435 | 1.00 | 0.00 |
| ATOM | 1130 | H | TYR | 1 | 542 | 22.957 | 68.275 | 37.510 | 1.00 | 0.00 |
| ATOM | 1131 | HH | TYR | 1 | 542 | 25.227 | 70.448 | 31.951 | 1.00 | 0.00 |
| ATOM | 1132 | N | ARG | 1 | 543 | 19.578 | 70.286 | 37.210 | 1.00 | 0.00 |
| ATOM | 1133 | CA | ARG | 1 | 543 | 18.724 | 70.753 | 38.288 | 1.00 | 0.00 |
| ATOM | 1134 | C | ARG | 1 | 543 | 17.730 | 71.831 | 37.825 | 1.00 | 0.00 |
| ATOM | 1135 | O | ARG | 1 | 543 | 16.876 | 71.559 | 36.980 | 1.00 | 0.00 |
| ATOM | 1136 | CB | ARG | 1 | 543 | 19.662 | 71.160 | 39.421 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1137 | CG | ARG | 1 | 543 | 19.219 | 70.805 | 40.834 | 1.00 | 0.00 |
| ATOM | 1138 | CD | ARG | 1 | 543 | 20.183 | 71.415 | 41.853 | 1.00 | 0.00 |
| ATOM | 1139 | NE | ARG | 1 | 543 | 20.189 | 72.854 | 41.622 | 1.00 | 0.00 |
| ATOM | 1140 | CZ | ARG | 1 | 543 | 19.158 | 73.567 | 42.118 | 1.00 | 0.00 |
| ATOM | 1141 | NH1 | ARG | 1 | 543 | 18.756 | 74.643 | 41.456 | 1.00 | 0.00 |
| ATOM | 1142 | NH2 | ARG | 1 | 543 | 18.554 | 73.153 | 43.227 | 1.00 | 0.00 |
| ATOM | 1143 | H | ARG | 1 | 543 | 20.075 | 70.951 | 36.654 | 1.00 | 0.00 |
| ATOM | 1144 | HE | ARG | 1 | 543 | 20.709 | 73.155 | 40.812 | 1.00 | 0.00 |
| ATOM | 1145 | 1HH1 | ARG | 1 | 543 | 18.100 | 75.303 | 41.819 | 1.00 | 0.00 |
| ATOM | 1146 | 2HH1 | ARG | 1 | 543 | 19.116 | 74.796 | 40.526 | 1.00 | 0.00 |
| ATOM | 1147 | 1HH2 | ARG | 1 | 543 | 17.690 | 73.523 | 43.577 | 1.00 | 0.00 |
| ATOM | 1148 | 2HH2 | ARG | 1 | 543 | 18.931 | 72.398 | 43.762 | 1.00 | 0.00 |
| ATOM | 1149 | N | LYS | 1 | 544 | 17.809 | 73.058 | 38.398 | 1.00 | 0.00 |
| ATOM | 1150 | CA | LYS | 1 | 544 | 16.969 | 74.161 | 37.889 | 1.00 | 0.00 |
| ATOM | 1151 | C | LYS | 1 | 544 | 17.595 | 75.562 | 37.999 | 1.00 | 0.00 |
| ATOM | 1152 | O | LYS | 1 | 544 | 17.936 | 76.058 | 39.076 | 1.00 | 0.00 |
| ATOM | 1153 | CB | LYS | 1 | 544 | 15.549 | 74.173 | 38.491 | 1.00 | 0.00 |
| ATOM | 1154 | CG | LYS | 1 | 544 | 14.550 | 73.281 | 37.734 | 1.00 | 0.00 |
| ATOM | 1155 | CD | LYS | 1 | 544 | 14.424 | 73.661 | 36.251 | 1.00 | 0.00 |
| ATOM | 1156 | CE | LYS | 1 | 544 | 13.864 | 72.560 | 35.339 | 1.00 | 0.00 |
| ATOM | 1157 | NZ | LYS | 1 | 544 | 14.812 | 71.451 | 35.222 | 1.00 | 0.00 |
| ATOM | 1158 | H | LYS | 1 | 544 | 18.591 | 73.318 | 38.972 | 1.00 | 0.00 |
| ATOM | 1159 | 1HZ | LYS | 1 | 544 | 15.712 | 71.621 | 35.714 | 1.00 | 0.00 |
| ATOM | 1160 | 2HZ | LYS | 1 | 544 | 14.379 | 70.596 | 35.625 | 1.00 | 0.00 |
| ATOM | 1161 | 3HZ | LYS | 1 | 544 | 14.992 | 71.196 | 34.231 | 1.00 | 0.00 |
| ATOM | 1162 | N | PRO | 1 | 545 | 17.742 | 76.210 | 36.807 | 1.00 | 0.00 |
| ATOM | 1163 | CA | PRO | 1 | 545 | 18.117 | 77.638 | 36.764 | 1.00 | 0.00 |
| ATOM | 1164 | C | PRO | 1 | 545 | 16.943 | 78.506 | 37.222 | 1.00 | 0.00 |
| ATOM | 1165 | O | PRO | 1 | 545 | 16.074 | 77.996 | 37.928 | 1.00 | 0.00 |
| ATOM | 1166 | CB | PRO | 1 | 545 | 18.505 | 77.814 | 35.290 | 1.00 | 0.00 |
| ATOM | 1167 | CG | PRO | 1 | 545 | 17.611 | 76.836 | 34.532 | 1.00 | 0.00 |
| ATOM | 1168 | CD | PRO | 1 | 545 | 17.550 | 75.642 | 35.475 | 1.00 | 0.00 |
| ATOM | 1169 | N | ASN | 1 | 546 | 16.924 | 79.787 | 36.814 | 1.00 | 0.00 |
| ATOM | 1170 | CA | ASN | 1 | 546 | 15.784 | 80.624 | 37.213 | 1.00 | 0.00 |
| ATOM | 1171 | C | ASN | 1 | 546 | 15.605 | 81.800 | 36.261 | 1.00 | 0.00 |
| ATOM | 1172 | O | ASN | 1 | 546 | 16.443 | 82.018 | 35.394 | 1.00 | 0.00 |
| ATOM | 1173 | CB | ASN | 1 | 546 | 15.945 | 81.086 | 38.675 | 1.00 | 0.00 |
| ATOM | 1174 | CG | ASN | 1 | 546 | 14.609 | 81.544 | 39.227 | 1.00 | 0.00 |
| ATOM | 1175 | OD1 | ASN | 1 | 546 | 13.546 | 81.250 | 38.694 | 1.00 | 0.00 |
| ATOM | 1176 | ND2 | ASN | 1 | 546 | 14.682 | 82.354 | 40.285 | 1.00 | 0.00 |
| ATOM | 1177 | H | ASN | 1 | 546 | 17.703 | 80.152 | 36.302 | 1.00 | 0.00 |
| ATOM | 1178 | 1HD2 | ASN | 1 | 546 | 13.838 | 82.720 | 40.678 | 1.00 | 0.00 |
| ATOM | 1179 | 2HD2 | ASN | 1 | 546 | 15.560 | 82.630 | 40.674 | 1.00 | 0.00 |
| ATOM | 1180 | N | GLY | 1 | 547 | 14.510 | 82.562 | 36.429 | 1.00 | 0.00 |
| ATOM | 1181 | CA | GLY | 1 | 547 | 14.372 | 83.804 | 35.670 | 1.00 | 0.00 |
| ATOM | 1182 | C | GLY | 1 | 547 | 15.218 | 84.921 | 36.251 | 1.00 | 0.00 |
| ATOM | 1183 | O | GLY | 1 | 547 | 14.741 | 85.841 | 36.914 | 1.00 | 0.00 |
| ATOM | 1184 | H | GLY | 1 | 547 | 13.842 | 82.337 | 37.137 | 1.00 | 0.00 |
| ATOM | 1185 | N | THR | 1 | 548 | 16.507 | 84.756 | 35.977 | 1.00 | 0.00 |
| ATOM | 1186 | CA | THR | 1 | 548 | 17.535 | 85.654 | 36.464 | 1.00 | 0.00 |
| ATOM | 1187 | C | THR | 1 | 548 | 18.697 | 85.468 | 35.515 | 1.00 | 0.00 |
| ATOM | 1188 | O | THR | 1 | 548 | 18.884 | 84.374 | 34.982 | 1.00 | 0.00 |
| ATOM | 1189 | CB | THR | 1 | 548 | 17.878 | 85.310 | 37.933 | 1.00 | 0.00 |
| ATOM | 1190 | OG1 | THR | 1 | 548 | 18.666 | 86.333 | 38.558 | 1.00 | 0.00 |
| ATOM | 1191 | CG2 | THR | 1 | 548 | 18.519 | 83.929 | 38.121 | 1.00 | 0.00 |
| ATOM | 1192 | H | THR | 1 | 548 | 16.804 | 84.002 | 35.392 | 1.00 | 0.00 |
| ATOM | 1193 | HG1 | THR | 1 | 548 | 19.565 | 86.036 | 38.441 | 1.00 | 0.00 |
| ATOM | 1194 | N | ASN | 1 | 549 | 19.420 | 86.581 | 35.312 | 1.00 | 0.00 |
| ATOM | 1195 | CA | ASN | 1 | 549 | 20.592 | 86.651 | 34.427 | 1.00 | 0.00 |
| ATOM | 1196 | C | ASN | 1 | 549 | 20.634 | 85.770 | 33.181 | 1.00 | 0.00 |
| ATOM | 1197 | O | ASN | 1 | 549 | 20.936 | 84.584 | 33.226 | 1.00 | 0.00 |
| ATOM | 1198 | CB | ASN | 1 | 549 | 21.889 | 86.500 | 35.221 | 1.00 | 0.00 |
| ATOM | 1199 | CG | ASN | 1 | 549 | 22.961 | 87.289 | 34.500 | 1.00 | 0.00 |
| ATOM | 1200 | OD1 | ASN | 1 | 549 | 22.887 | 88.504 | 34.382 | 1.00 | 0.00 |
| ATOM | 1201 | ND2 | ASN | 1 | 549 | 23.958 | 86.559 | 34.004 | 1.00 | 0.00 |
| ATOM | 1202 | H | ASN | 1 | 549 | 19.148 | 87.393 | 35.826 | 1.00 | 0.00 |
| ATOM | 1203 | 1HD2 | ASN | 1 | 549 | 24.674 | 87.020 | 33.479 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1204 | 2HD2 | ASN | 1 | 549 | 23.944 | 85.566 | 34.151 | 1.00 | 0.00 |
| ATOM | 1205 | N | PRO | 1 | 550 | 20.326 | 86.400 | 32.030 | 1.00 | 0.00 |
| ATOM | 1206 | CA | PRO | 1 | 550 | 20.393 | 85.645 | 30.774 | 1.00 | 0.00 |
| ATOM | 1207 | C | PRO | 1 | 550 | 21.822 | 85.253 | 30.413 | 1.00 | 0.00 |
| ATOM | 1208 | O | PRO | 1 | 550 | 22.788 | 85.652 | 31.055 | 1.00 | 0.00 |
| ATOM | 1209 | CB | PRO | 1 | 550 | 19.752 | 86.627 | 29.785 | 1.00 | 0.00 |
| ATOM | 1210 | CG | PRO | 1 | 550 | 20.050 | 88.016 | 30.352 | 1.00 | 0.00 |
| ATOM | 1211 | CD | PRO | 1 | 550 | 19.943 | 87.795 | 31.856 | 1.00 | 0.00 |
| ATOM | 1212 | N | GLY | 1 | 551 | 21.912 | 84.448 | 29.343 | 1.00 | 0.00 |
| ATOM | 1213 | CA | GLY | 1 | 551 | 23.229 | 84.216 | 28.765 | 1.00 | 0.00 |
| ATOM | 1214 | C | GLY | 1 | 551 | 23.394 | 82.772 | 28.330 | 1.00 | 0.00 |
| ATOM | 1215 | 1OCT | GLY | 1 | 551 | 22.524 | 82.235 | 27.651 | 1.00 | 0.00 |
| ATOM | 1216 | 2OCT | GLY | 1 | 551 | 24.388 | 82.150 | 28.679 | 1.00 | 0.00 |
| ATOM | 1217 | H | GLY | 1 | 551 | 21.108 | 84.092 | 28.872 | 1.00 | 0.00 |
| ATOM | 1218 | N | VAL | 2 | 661 | 27.598 | 80.303 | 30.863 | 1.00 | 0.00 |
| ATOM | 1219 | CA | VAL | 2 | 661 | 26.263 | 79.728 | 30.969 | 1.00 | 0.00 |
| ATOM | 1220 | C | VAL | 2 | 661 | 25.556 | 80.497 | 32.068 | 1.00 | 0.00 |
| ATOM | 1221 | O | VAL | 2 | 661 | 25.467 | 80.081 | 33.217 | 1.00 | 0.00 |
| ATOM | 1222 | CB | VAL | 2 | 661 | 26.370 | 78.202 | 31.202 | 1.00 | 0.00 |
| ATOM | 1223 | CG1 | VAL | 2 | 661 | 27.312 | 77.804 | 32.348 | 1.00 | 0.00 |
| ATOM | 1224 | CG2 | VAL | 2 | 661 | 24.986 | 77.549 | 31.304 | 1.00 | 0.00 |
| ATOM | 1225 | 1HT | VAL | 2 | 661 | 28.373 | 79.662 | 30.659 | 1.00 | 0.00 |
| ATOM | 1226 | 2HT | VAL | 2 | 661 | 27.567 | 81.082 | 30.178 | 1.00 | 0.00 |
| ATOM | 1227 | 3HT | VAL | 2 | 661 | 27.807 | 80.852 | 31.727 | 1.00 | 0.00 |
| ATOM | 1228 | N | GLU | 2 | 662 | 25.126 | 81.679 | 31.668 | 1.00 | 0.00 |
| ATOM | 1229 | CA | GLU | 2 | 662 | 24.988 | 82.716 | 32.681 | 1.00 | 0.00 |
| ATOM | 1230 | C | GLU | 2 | 662 | 23.622 | 82.747 | 33.349 | 1.00 | 0.00 |
| ATOM | 1231 | O | GLU | 2 | 662 | 23.418 | 83.336 | 34.410 | 1.00 | 0.00 |
| ATOM | 1232 | CB | GLU | 2 | 662 | 25.433 | 84.047 | 32.058 | 1.00 | 0.00 |
| ATOM | 1233 | CG | GLU | 2 | 662 | 26.956 | 84.230 | 31.848 | 1.00 | 0.00 |
| ATOM | 1234 | CD | GLU | 2 | 662 | 27.616 | 83.112 | 31.041 | 1.00 | 0.00 |
| ATOM | 1235 | OE1 | GLU | 2 | 662 | 28.591 | 82.529 | 31.503 | 1.00 | 0.00 |
| ATOM | 1236 | OE2 | GLU | 2 | 662 | 27.150 | 82.758 | 29.961 | 1.00 | 0.00 |
| ATOM | 1237 | H | GLU | 2 | 662 | 25.088 | 81.927 | 30.698 | 1.00 | 0.00 |
| ATOM | 1238 | N | ARG | 2 | 663 | 22.711 | 82.002 | 32.703 | 1.00 | 0.00 |
| ATOM | 1239 | CA | ARG | 2 | 663 | 21.528 | 81.518 | 33.404 | 1.00 | 0.00 |
| ATOM | 1240 | C | ARG | 2 | 663 | 21.879 | 80.481 | 34.467 | 1.00 | 0.00 |
| ATOM | 1241 | O | ARG | 2 | 663 | 21.905 | 79.271 | 34.258 | 1.00 | 0.00 |
| ATOM | 1242 | CB | ARG | 2 | 663 | 20.441 | 81.050 | 32.412 | 1.00 | 0.00 |
| ATOM | 1243 | CG | ARG | 2 | 663 | 20.705 | 79.852 | 31.476 | 1.00 | 0.00 |
| ATOM | 1244 | CD | ARG | 2 | 663 | 21.664 | 80.072 | 30.298 | 1.00 | 0.00 |
| ATOM | 1245 | NE | ARG | 2 | 663 | 21.777 | 78.845 | 29.506 | 1.00 | 0.00 |
| ATOM | 1246 | CZ | ARG | 2 | 663 | 22.668 | 78.713 | 28.500 | 1.00 | 0.00 |
| ATOM | 1247 | NH1 | ARG | 2 | 663 | 23.491 | 79.696 | 28.194 | 1.00 | 0.00 |
| ATOM | 1248 | NH2 | ARG | 2 | 663 | 22.699 | 77.584 | 27.805 | 1.00 | 0.00 |
| ATOM | 1249 | H | ARG | 2 | 663 | 22.936 | 81.716 | 31.777 | 1.00 | 0.00 |
| ATOM | 1250 | HE | ARG | 2 | 663 | 21.086 | 78.137 | 29.661 | 1.00 | 0.00 |
| ATOM | 1251 | 1HH1 | ARG | 2 | 663 | 24.209 | 79.607 | 27.508 | 1.00 | 0.00 |
| ATOM | 1252 | 2HH1 | ARG | 2 | 663 | 23.405 | 80.608 | 28.630 | 1.00 | 0.00 |
| ATOM | 1253 | 1HH2 | ARG | 2 | 663 | 23.351 | 77.465 | 27.057 | 1.00 | 0.00 |
| ATOM | 1254 | 2HH2 | ARG | 2 | 663 | 22.046 | 76.846 | 27.993 | 1.00 | 0.00 |
| ATOM | 1255 | N | MET | 2 | 664 | 22.200 | 81.036 | 35.642 | 1.00 | 0.00 |
| ATOM | 1256 | CA | MET | 2 | 664 | 22.810 | 80.216 | 36.689 | 1.00 | 0.00 |
| ATOM | 1257 | C | MET | 2 | 664 | 21.896 | 79.254 | 37.440 | 1.00 | 0.00 |
| ATOM | 1258 | O | MET | 2 | 664 | 20.702 | 79.490 | 37.616 | 1.00 | 0.00 |
| ATOM | 1259 | CB | MET | 2 | 664 | 23.575 | 81.119 | 37.661 | 1.00 | 0.00 |
| ATOM | 1260 | CG | MET | 2 | 664 | 22.690 | 82.057 | 38.488 | 1.00 | 0.00 |
| ATOM | 1261 | SD | MET | 2 | 664 | 23.644 | 83.095 | 39.604 | 1.00 | 0.00 |
| ATOM | 1262 | CE | MET | 2 | 664 | 24.466 | 81.779 | 40.517 | 1.00 | 0.00 |
| ATOM | 1263 | H | MET | 2 | 664 | 22.218 | 82.039 | 35.656 | 1.00 | 0.00 |
| ATOM | 1264 | N | GLU | 2 | 665 | 22.556 | 78.184 | 37.901 | 1.00 | 0.00 |
| ATOM | 1265 | CA | GLU | 2 | 665 | 21.973 | 77.302 | 38.915 | 1.00 | 0.00 |
| ATOM | 1266 | C | GLU | 2 | 665 | 22.267 | 77.781 | 40.329 | 1.00 | 0.00 |
| ATOM | 1267 | O | GLU | 2 | 665 | 22.769 | 78.869 | 40.570 | 1.00 | 0.00 |
| ATOM | 1268 | CB | GLU | 2 | 665 | 22.570 | 75.910 | 38.755 | 1.00 | 0.00 |
| ATOM | 1269 | CG | GLU | 2 | 665 | 22.002 | 75.104 | 37.596 | 1.00 | 0.00 |
| ATOM | 1270 | CD | GLU | 2 | 665 | 20.719 | 74.408 | 37.989 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1271 | OE1 | GLU | 2 | 665 | 20.096 | 73.819 | 37.118 | 1.00 | 0.00 |
| ATOM | 1272 | OE2 | GLU | 2 | 665 | 20.326 | 74.427 | 39.152 | 1.00 | 0.00 |
| ATOM | 1273 | H | GLU | 2 | 665 | 23.513 | 78.100 | 37.627 | 1.00 | 0.00 |
| ATOM | 1274 | N | SER | 2 | 666 | 22.008 | 76.912 | 41.322 | 1.00 | 0.00 |
| ATOM | 1275 | CA | SER | 2 | 666 | 22.509 | 77.312 | 42.643 | 1.00 | 0.00 |
| ATOM | 1276 | C | SER | 2 | 666 | 23.955 | 76.931 | 43.008 | 1.00 | 0.00 |
| ATOM | 1277 | O | SER | 2 | 666 | 24.791 | 77.823 | 43.161 | 1.00 | 0.00 |
| ATOM | 1278 | CB | SER | 2 | 666 | 21.457 | 77.014 | 43.724 | 1.00 | 0.00 |
| ATOM | 1279 | OG | SER | 2 | 666 | 20.605 | 75.940 | 43.273 | 1.00 | 0.00 |
| ATOM | 1280 | H | SER | 2 | 666 | 21.617 | 76.002 | 41.195 | 1.00 | 0.00 |
| ATOM | 1281 | HG | SER | 2 | 666 | 19.780 | 76.370 | 43.045 | 1.00 | 0.00 |
| ATOM | 1282 | N | PRO | 2 | 667 | 24.249 | 75.606 | 43.156 | 1.00 | 0.00 |
| ATOM | 1283 | CA | PRO | 2 | 667 | 25.596 | 75.246 | 43.590 | 1.00 | 0.00 |
| ATOM | 1284 | C | PRO | 2 | 667 | 26.467 | 74.842 | 42.408 | 1.00 | 0.00 |
| ATOM | 1285 | O | PRO | 2 | 667 | 26.149 | 75.082 | 41.242 | 1.00 | 0.00 |
| ATOM | 1286 | CB | PRO | 2 | 667 | 25.278 | 74.098 | 44.552 | 1.00 | 0.00 |
| ATOM | 1287 | CG | PRO | 2 | 667 | 24.076 | 73.372 | 43.941 | 1.00 | 0.00 |
| ATOM | 1288 | CD | PRO | 2 | 667 | 23.408 | 74.413 | 43.044 | 1.00 | 0.00 |
| ATOM | 1289 | N | ILE | 2 | 668 | 27.586 | 74.199 | 42.767 | 1.00 | 0.00 |
| ATOM | 1290 | CA | ILE | 2 | 668 | 28.525 | 73.667 | 41.784 | 1.00 | 0.00 |
| ATOM | 1291 | C | ILE | 2 | 668 | 29.181 | 72.428 | 42.397 | 1.00 | 0.00 |
| ATOM | 1292 | O | ILE | 2 | 668 | 28.803 | 72.017 | 43.492 | 1.00 | 0.00 |
| ATOM | 1293 | CB | ILE | 2 | 668 | 29.492 | 74.803 | 41.376 | 1.00 | 0.00 |
| ATOM | 1294 | CG1 | ILE | 2 | 668 | 30.291 | 74.533 | 40.096 | 1.00 | 0.00 |
| ATOM | 1295 | CG2 | ILE | 2 | 668 | 30.392 | 75.207 | 42.554 | 1.00 | 0.00 |
| ATOM | 1296 | CD1 | ILE | 2 | 668 | 31.169 | 75.711 | 39.673 | 1.00 | 0.00 |
| ATOM | 1297 | H | ILE | 2 | 668 | 27.817 | 74.032 | 43.729 | 1.00 | 0.00 |
| ATOM | 1298 | N | ASP | 2 | 669 | 30.171 | 71.823 | 41.725 | 1.00 | 0.00 |
| ATOM | 1299 | CA | ASP | 2 | 669 | 31.112 | 70.987 | 42.470 | 1.00 | 0.00 |
| ATOM | 1300 | C | ASP | 2 | 669 | 32.413 | 71.757 | 42.646 | 1.00 | 0.00 |
| ATOM | 1301 | O | ASP | 2 | 669 | 33.355 | 71.639 | 41.866 | 1.00 | 0.00 |
| ATOM | 1302 | CB | ASP | 2 | 669 | 31.317 | 69.654 | 41.727 | 1.00 | 0.00 |
| ATOM | 1303 | CG | ASP | 2 | 669 | 32.130 | 68.609 | 42.487 | 1.00 | 0.00 |
| ATOM | 1304 | OD1 | ASP | 2 | 669 | 31.638 | 67.512 | 42.712 | 1.00 | 0.00 |
| ATOM | 1305 | OD2 | ASP | 2 | 669 | 33.277 | 68.845 | 42.824 | 1.00 | 0.00 |
| ATOM | 1306 | H | ASP | 2 | 669 | 30.406 | 72.058 | 40.785 | 1.00 | 0.00 |
| ATOM | 1307 | N | SER | 2 | 670 | 32.429 | 72.593 | 43.691 | 1.00 | 0.00 |
| ATOM | 1308 | CA | SER | 2 | 670 | 33.782 | 72.929 | 44.123 | 1.00 | 0.00 |
| ATOM | 1309 | C | SER | 2 | 670 | 34.070 | 72.069 | 45.326 | 1.00 | 0.00 |
| ATOM | 1310 | O | SER | 2 | 670 | 33.161 | 71.429 | 45.856 | 1.00 | 0.00 |
| ATOM | 1311 | CB | SER | 2 | 670 | 33.990 | 74.424 | 44.396 | 1.00 | 0.00 |
| ATOM | 1312 | OG | SER | 2 | 670 | 35.391 | 74.750 | 44.269 | 1.00 | 0.00 |
| ATOM | 1313 | H | SER | 2 | 670 | 31.641 | 72.614 | 44.306 | 1.00 | 0.00 |
| ATOM | 1314 | HG | SER | 2 | 670 | 35.543 | 74.887 | 43.337 | 1.00 | 0.00 |
| ATOM | 1315 | N | ALA | 2 | 671 | 35.353 | 72.030 | 45.714 | 1.00 | 0.00 |
| ATOM | 1316 | CA | ALA | 2 | 671 | 35.787 | 70.958 | 46.612 | 1.00 | 0.00 |
| ATOM | 1317 | C | ALA | 2 | 671 | 34.894 | 70.727 | 47.821 | 1.00 | 0.00 |
| ATOM | 1318 | O | ALA | 2 | 671 | 34.607 | 69.592 | 48.217 | 1.00 | 0.00 |
| ATOM | 1319 | CB | ALA | 2 | 671 | 37.216 | 71.211 | 47.095 | 1.00 | 0.00 |
| ATOM | 1320 | H | ALA | 2 | 671 | 35.970 | 72.721 | 45.334 | 1.00 | 0.00 |
| ATOM | 1321 | N | ASP | 2 | 672 | 34.484 | 71.881 | 48.360 | 1.00 | 0.00 |
| ATOM | 1322 | CA | ASP | 2 | 672 | 33.662 | 71.994 | 49.554 | 1.00 | 0.00 |
| ATOM | 1323 | C | ASP | 2 | 672 | 32.192 | 71.630 | 49.402 | 1.00 | 0.00 |
| ATOM | 1324 | O | ASP | 2 | 672 | 31.609 | 71.007 | 50.280 | 1.00 | 0.00 |
| ATOM | 1325 | CB | ASP | 2 | 672 | 33.851 | 73.407 | 50.136 | 1.00 | 0.00 |
| ATOM | 1326 | CG | ASP | 2 | 672 | 33.226 | 74.521 | 49.291 | 1.00 | 0.00 |
| ATOM | 1327 | OD1 | ASP | 2 | 672 | 33.056 | 74.399 | 48.083 | 1.00 | 0.00 |
| ATOM | 1328 | OD2 | ASP | 2 | 672 | 32.847 | 75.536 | 49.848 | 1.00 | 0.00 |
| ATOM | 1329 | H | ASP | 2 | 672 | 34.663 | 72.741 | 47.874 | 1.00 | 0.00 |
| ATOM | 1330 | N | ASP | 2 | 673 | 31.611 | 72.031 | 48.264 | 1.00 | 0.00 |
| ATOM | 1331 | CA | ASP | 2 | 673 | 30.153 | 72.026 | 48.133 | 1.00 | 0.00 |
| ATOM | 1332 | C | ASP | 2 | 673 | 29.400 | 70.805 | 48.581 | 1.00 | 0.00 |
| ATOM | 1333 | O | ASP | 2 | 673 | 28.325 | 70.874 | 49.170 | 1.00 | 0.00 |
| ATOM | 1334 | CB | ASP | 2 | 673 | 29.715 | 72.385 | 46.718 | 1.00 | 0.00 |
| ATOM | 1335 | CG | ASP | 2 | 673 | 29.455 | 73.868 | 46.695 | 1.00 | 0.00 |
| ATOM | 1336 | OD1 | ASP | 2 | 673 | 30.222 | 74.599 | 46.087 | 1.00 | 0.00 |
| ATOM | 1337 | OD2 | ASP | 2 | 673 | 28.512 | 74.326 | 47.330 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1338 | H | ASP | 2 | 673 | 32.166 | 72.591 | 47.651 | 1.00 | 0.00 |
| ATOM | 1339 | N | LEU | 2 | 674 | 29.995 | 69.655 | 48.259 | 1.00 | 0.00 |
| ATOM | 1340 | CA | LEU | 2 | 674 | 29.339 | 68.380 | 48.593 | 1.00 | 0.00 |
| ATOM | 1341 | C | LEU | 2 | 674 | 29.158 | 68.130 | 50.094 | 1.00 | 0.00 |
| ATOM | 1342 | O | LEU | 2 | 674 | 28.239 | 67.471 | 50.591 | 1.00 | 0.00 |
| ATOM | 1343 | CB | LEU | 2 | 674 | 30.091 | 67.226 | 47.931 | 1.00 | 0.00 |
| ATOM | 1344 | CG | LEU | 2 | 674 | 30.315 | 67.407 | 46.425 | 1.00 | 0.00 |
| ATOM | 1345 | CD1 | LEU | 2 | 674 | 31.186 | 66.288 | 45.855 | 1.00 | 0.00 |
| ATOM | 1346 | CD2 | LEU | 2 | 674 | 29.007 | 67.564 | 45.645 | 1.00 | 0.00 |
| ATOM | 1347 | H | LEU | 2 | 674 | 30.934 | 69.748 | 47.921 | 1.00 | 0.00 |
| ATOM | 1348 | N | ALA | 2 | 675 | 30.107 | 68.745 | 50.823 | 1.00 | 0.00 |
| ATOM | 1349 | CA | ALA | 2 | 675 | 29.893 | 68.948 | 52.247 | 1.00 | 0.00 |
| ATOM | 1350 | C | ALA | 2 | 675 | 28.977 | 70.126 | 52.547 | 1.00 | 0.00 |
| ATOM | 1351 | O | ALA | 2 | 675 | 27.881 | 69.949 | 53.081 | 1.00 | 0.00 |
| ATOM | 1352 | CB | ALA | 2 | 675 | 31.229 | 69.112 | 52.978 | 1.00 | 0.00 |
| ATOM | 1353 | H | ALA | 2 | 675 | 30.804 | 69.271 | 50.333 | 1.00 | 0.00 |
| ATOM | 1354 | N | LYS | 2 | 676 | 29.480 | 71.327 | 52.195 | 1.00 | 0.00 |
| ATOM | 1355 | CA | LYS | 2 | 676 | 28.894 | 72.557 | 52.738 | 1.00 | 0.00 |
| ATOM | 1356 | C | LYS | 2 | 676 | 27.471 | 72.898 | 52.342 | 1.00 | 0.00 |
| ATOM | 1357 | O | LYS | 2 | 676 | 26.668 | 73.386 | 53.138 | 1.00 | 0.00 |
| ATOM | 1358 | CB | LYS | 2 | 676 | 29.849 | 73.760 | 52.585 | 1.00 | 0.00 |
| ATOM | 1359 | CG | LYS | 2 | 676 | 30.206 | 74.357 | 51.208 | 1.00 | 0.00 |
| ATOM | 1360 | CD | LYS | 2 | 676 | 29.203 | 75.324 | 50.556 | 1.00 | 0.00 |
| ATOM | 1361 | CE | LYS | 2 | 676 | 29.827 | 76.426 | 49.668 | 1.00 | 0.00 |
| ATOM | 1362 | NZ | LYS | 2 | 676 | 30.612 | 75.894 | 48.542 | 1.00 | 0.00 |
| ATOM | 1363 | H | LYS | 2 | 676 | 30.342 | 71.342 | 51.682 | 1.00 | 0.00 |
| ATOM | 1364 | 1HZ | LYS | 2 | 676 | 31.383 | 75.271 | 48.867 | 1.00 | 0.00 |
| ATOM | 1365 | 2HZ | LYS | 2 | 676 | 30.017 | 75.377 | 47.866 | 1.00 | 0.00 |
| ATOM | 1366 | 3HZ | LYS | 2 | 676 | 31.097 | 76.655 | 48.032 | 1.00 | 0.00 |
| ATOM | 1367 | N | GLN | 2 | 677 | 27.165 | 72.614 | 51.071 | 1.00 | 0.00 |
| ATOM | 1368 | CA | GLN | 2 | 677 | 25.790 | 72.829 | 50.634 | 1.00 | 0.00 |
| ATOM | 1369 | C | GLN | 2 | 677 | 24.861 | 71.693 | 51.029 | 1.00 | 0.00 |
| ATOM | 1370 | O | GLN | 2 | 677 | 24.418 | 70.900 | 50.208 | 1.00 | 0.00 |
| ATOM | 1371 | CB | GLN | 2 | 677 | 25.727 | 73.079 | 49.126 | 1.00 | 0.00 |
| ATOM | 1372 | CG | GLN | 2 | 677 | 24.646 | 74.089 | 48.728 | 1.00 | 0.00 |
| ATOM | 1373 | CD | GLN | 2 | 677 | 25.132 | 75.495 | 49.029 | 1.00 | 0.00 |
| ATOM | 1374 | OE1 | GLN | 2 | 677 | 24.853 | 76.093 | 50.068 | 1.00 | 0.00 |
| ATOM | 1375 | NE2 | GLN | 2 | 677 | 25.892 | 75.992 | 48.046 | 1.00 | 0.00 |
| ATOM | 1376 | H | GLN | 2 | 677 | 27.849 | 72.133 | 50.522 | 1.00 | 0.00 |
| ATOM | 1377 | 1HE2 | GLN | 2 | 677 | 26.290 | 76.905 | 48.108 | 1.00 | 0.00 |
| ATOM | 1378 | 2HE2 | GLN | 2 | 677 | 26.081 | 75.431 | 47.239 | 1.00 | 0.00 |
| ATOM | 1379 | N | THR | 2 | 678 | 24.584 | 71.652 | 52.345 | 1.00 | 0.00 |
| ATOM | 1380 | CA | THR | 2 | 678 | 23.696 | 70.674 | 52.996 | 1.00 | 0.00 |
| ATOM | 1381 | C | THR | 2 | 678 | 22.307 | 70.572 | 52.369 | 1.00 | 0.00 |
| ATOM | 1382 | O | THR | 2 | 678 | 21.312 | 71.089 | 52.874 | 1.00 | 0.00 |
| ATOM | 1383 | CB | THR | 2 | 678 | 23.648 | 70.947 | 54.530 | 1.00 | 0.00 |
| ATOM | 1384 | OG1 | THR | 2 | 678 | 22.771 | 70.051 | 55.251 | 1.00 | 0.00 |
| ATOM | 1385 | CG2 | THR | 2 | 678 | 23.313 | 72.408 | 54.862 | 1.00 | 0.00 |
| ATOM | 1386 | H | THR | 2 | 678 | 24.992 | 72.379 | 52.897 | 1.00 | 0.00 |
| ATOM | 1387 | HG1 | THR | 2 | 678 | 21.971 | 70.016 | 54.732 | 1.00 | 0.00 |
| ATOM | 1388 | N | LYS | 2 | 679 | 22.292 | 69.841 | 51.247 | 1.00 | 0.00 |
| ATOM | 1389 | CA | LYS | 2 | 679 | 21.134 | 69.696 | 50.371 | 1.00 | 0.00 |
| ATOM | 1390 | C | LYS | 2 | 679 | 21.482 | 68.810 | 49.194 | 1.00 | 0.00 |
| ATOM | 1391 | O | LYS | 2 | 679 | 20.696 | 67.953 | 48.805 | 1.00 | 0.00 |
| ATOM | 1392 | CB | LYS | 2 | 679 | 20.625 | 71.036 | 49.807 | 1.00 | 0.00 |
| ATOM | 1393 | CG | LYS | 2 | 679 | 19.215 | 70.982 | 49.191 | 1.00 | 0.00 |
| ATOM | 1394 | CD | LYS | 2 | 679 | 18.862 | 72.270 | 48.438 | 1.00 | 0.00 |
| ATOM | 1395 | CE | LYS | 2 | 679 | 17.375 | 72.479 | 48.105 | 1.00 | 0.00 |
| ATOM | 1396 | NZ | LYS | 2 | 679 | 16.836 | 71.473 | 47.181 | 1.00 | 0.00 |
| ATOM | 1397 | H | LYS | 2 | 679 | 23.178 | 69.488 | 50.944 | 1.00 | 0.00 |
| ATOM | 1398 | 1HZ | LYS | 2 | 679 | 17.529 | 70.981 | 46.593 | 1.00 | 0.00 |
| ATOM | 1399 | 2HZ | LYS | 2 | 679 | 16.220 | 70.779 | 47.629 | 1.00 | 0.00 |
| ATOM | 1400 | 3HZ | LYS | 2 | 679 | 16.235 | 71.952 | 46.475 | 1.00 | 0.00 |
| ATOM | 1401 | N | ILE | 2 | 680 | 22.657 | 69.099 | 48.623 | 1.00 | 0.00 |
| ATOM | 1402 | CA | ILE | 2 | 680 | 22.945 | 68.624 | 47.273 | 1.00 | 0.00 |
| ATOM | 1403 | C | ILE | 2 | 680 | 23.012 | 67.111 | 47.066 | 1.00 | 0.00 |
| ATOM | 1404 | O | ILE | 2 | 680 | 24.036 | 66.447 | 47.222 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1405 | CB | ILE | 2 | 680 | 24.183 | 69.371 | 46.724 | 1.00 | 0.00 |
| ATOM | 1406 | CG1 | ILE | 2 | 680 | 24.464 | 69.050 | 45.250 | 1.00 | 0.00 |
| ATOM | 1407 | CG2 | ILE | 2 | 680 | 25.429 | 69.134 | 47.596 | 1.00 | 0.00 |
| ATOM | 1408 | CD1 | ILE | 2 | 680 | 25.683 | 69.788 | 44.692 | 1.00 | 0.00 |
| ATOM | 1409 | H | ILE | 2 | 680 | 23.231 | 69.823 | 49.006 | 1.00 | 0.00 |
| ATOM | 1410 | N | GLU | 2 | 681 | 21.878 | 66.555 | 46.631 | 1.00 | 0.00 |
| ATOM | 1411 | CA | GLU | 2 | 681 | 22.089 | 65.263 | 45.994 | 1.00 | 0.00 |
| ATOM | 1412 | C | GLU | 2 | 681 | 22.545 | 65.426 | 44.565 | 1.00 | 0.00 |
| ATOM | 1413 | O | GLU | 2 | 681 | 21.767 | 65.563 | 43.617 | 1.00 | 0.00 |
| ATOM | 1414 | CB | GLU | 2 | 681 | 20.903 | 64.305 | 46.076 | 1.00 | 0.00 |
| ATOM | 1415 | CG | GLU | 2 | 681 | 21.433 | 62.907 | 45.719 | 1.00 | 0.00 |
| ATOM | 1416 | CD | GLU | 2 | 681 | 20.362 | 61.839 | 45.649 | 1.00 | 0.00 |
| ATOM | 1417 | OE1 | GLU | 2 | 681 | 20.691 | 60.688 | 45.404 | 1.00 | 0.00 |
| ATOM | 1418 | OE2 | GLU | 2 | 681 | 19.191 | 62.128 | 45.823 | 1.00 | 0.00 |
| ATOM | 1419 | H | GLU | 2 | 681 | 21.056 | 67.106 | 46.534 | 1.00 | 0.00 |
| ATOM | 1420 | N | TYR | 2 | 682 | 23.880 | 65.428 | 44.455 | 1.00 | 0.00 |
| ATOM | 1421 | CA | TYR | 2 | 682 | 24.428 | 65.288 | 43.118 | 1.00 | 0.00 |
| ATOM | 1422 | C | TYR | 2 | 682 | 24.213 | 63.876 | 42.616 | 1.00 | 0.00 |
| ATOM | 1423 | O | TYR | 2 | 682 | 24.173 | 62.909 | 43.385 | 1.00 | 0.00 |
| ATOM | 1424 | CB | TYR | 2 | 682 | 25.876 | 65.816 | 43.046 | 1.00 | 0.00 |
| ATOM | 1425 | CG | TYR | 2 | 682 | 26.946 | 64.777 | 43.313 | 1.00 | 0.00 |
| ATOM | 1426 | CD1 | TYR | 2 | 682 | 27.545 | 64.157 | 42.200 | 1.00 | 0.00 |
| ATOM | 1427 | CD2 | TYR | 2 | 682 | 27.335 | 64.471 | 44.633 | 1.00 | 0.00 |
| ATOM | 1428 | CE1 | TYR | 2 | 682 | 28.564 | 63.216 | 42.401 | 1.00 | 0.00 |
| ATOM | 1429 | CE2 | TYR | 2 | 682 | 28.363 | 63.533 | 44.837 | 1.00 | 0.00 |
| ATOM | 1430 | CZ | TYR | 2 | 682 | 28.958 | 62.912 | 43.717 | 1.00 | 0.00 |
| ATOM | 1431 | OH | TYR | 2 | 682 | 29.946 | 61.957 | 43.904 | 1.00 | 0.00 |
| ATOM | 1432 | H | TYR | 2 | 682 | 24.399 | 65.292 | 45.295 | 1.00 | 0.00 |
| ATOM | 1433 | HH | TYR | 2 | 682 | 30.344 | 62.051 | 44.774 | 1.00 | 0.00 |
| ATOM | 1434 | N | GLY | 2 | 683 | 23.971 | 63.830 | 41.322 | 1.00 | 0.00 |
| ATOM | 1435 | CA | GLY | 2 | 683 | 23.567 | 62.532 | 40.844 | 1.00 | 0.00 |
| ATOM | 1436 | C | GLY | 2 | 683 | 24.668 | 61.833 | 40.118 | 1.00 | 0.00 |
| ATOM | 1437 | O | GLY | 2 | 683 | 25.860 | 62.091 | 40.299 | 1.00 | 0.00 |
| ATOM | 1438 | H | GLY | 2 | 683 | 24.259 | 64.560 | 40.706 | 1.00 | 0.00 |
| ATOM | 1439 | N | ALA | 2 | 684 | 24.139 | 60.974 | 39.248 | 1.00 | 0.00 |
| ATOM | 1440 | CA | ALA | 2 | 684 | 24.823 | 60.216 | 38.216 | 1.00 | 0.00 |
| ATOM | 1441 | C | ALA | 2 | 684 | 23.777 | 59.263 | 37.703 | 1.00 | 0.00 |
| ATOM | 1442 | O | ALA | 2 | 684 | 22.918 | 58.777 | 38.450 | 1.00 | 0.00 |
| ATOM | 1443 | CB | ALA | 2 | 684 | 25.997 | 59.396 | 38.746 | 1.00 | 0.00 |
| ATOM | 1444 | H | ALA | 2 | 684 | 23.143 | 60.895 | 39.258 | 1.00 | 0.00 |
| ATOM | 1445 | N | VAL | 2 | 685 | 23.856 | 59.023 | 36.390 | 1.00 | 0.00 |
| ATOM | 1446 | CA | VAL | 2 | 685 | 22.980 | 58.034 | 35.757 | 1.00 | 0.00 |
| ATOM | 1447 | C | VAL | 2 | 685 | 23.389 | 56.658 | 36.214 | 1.00 | 0.00 |
| ATOM | 1448 | O | VAL | 2 | 685 | 24.462 | 56.546 | 36.812 | 1.00 | 0.00 |
| ATOM | 1449 | CB | VAL | 2 | 685 | 23.037 | 58.156 | 34.233 | 1.00 | 0.00 |
| ATOM | 1450 | CG1 | VAL | 2 | 685 | 22.668 | 59.583 | 33.856 | 1.00 | 0.00 |
| ATOM | 1451 | CG2 | VAL | 2 | 685 | 24.383 | 57.739 | 33.631 | 1.00 | 0.00 |
| ATOM | 1452 | H | VAL | 2 | 685 | 24.583 | 59.488 | 35.893 | 1.00 | 0.00 |
| ATOM | 1453 | N | GLU | 2 | 686 | 22.523 | 55.674 | 35.975 | 1.00 | 0.00 |
| ATOM | 1454 | CA | GLU | 2 | 686 | 22.859 | 54.388 | 36.583 | 1.00 | 0.00 |
| ATOM | 1455 | C | GLU | 2 | 686 | 24.055 | 53.719 | 35.929 | 1.00 | 0.00 |
| ATOM | 1456 | O | GLU | 2 | 686 | 24.981 | 53.192 | 36.559 | 1.00 | 0.00 |
| ATOM | 1457 | CB | GLU | 2 | 686 | 21.602 | 53.511 | 36.601 | 1.00 | 0.00 |
| ATOM | 1458 | CG | GLU | 2 | 686 | 21.046 | 53.173 | 37.998 | 1.00 | 0.00 |
| ATOM | 1459 | CD | GLU | 2 | 686 | 20.491 | 54.358 | 38.794 | 1.00 | 0.00 |
| ATOM | 1460 | OE1 | GLU | 2 | 686 | 20.766 | 55.511 | 38.494 | 1.00 | 0.00 |
| ATOM | 1461 | OE2 | GLU | 2 | 686 | 19.757 | 54.139 | 39.752 | 1.00 | 0.00 |
| ATOM | 1462 | H | GLU | 2 | 686 | 21.803 | 55.748 | 35.284 | 1.00 | 0.00 |
| ATOM | 1463 | N | ASP | 2 | 687 | 24.039 | 53.849 | 34.595 | 1.00 | 0.00 |
| ATOM | 1464 | CA | ASP | 2 | 687 | 25.102 | 53.265 | 33.769 | 1.00 | 0.00 |
| ATOM | 1465 | C | ASP | 2 | 687 | 26.520 | 53.782 | 34.061 | 1.00 | 0.00 |
| ATOM | 1466 | O | ASP | 2 | 687 | 27.550 | 53.252 | 33.631 | 1.00 | 0.00 |
| ATOM | 1467 | CB | ASP | 2 | 687 | 24.701 | 53.397 | 32.288 | 1.00 | 0.00 |
| ATOM | 1468 | CG | ASP | 2 | 687 | 23.210 | 53.104 | 32.120 | 1.00 | 0.00 |
| ATOM | 1469 | OD1 | ASP | 2 | 687 | 22.424 | 54.039 | 32.036 | 1.00 | 0.00 |
| ATOM | 1470 | OD2 | ASP | 2 | 687 | 22.804 | 51.951 | 32.115 | 1.00 | 0.00 |
| ATOM | 1471 | H | ASP | 2 | 687 | 23.221 | 54.260 | 34.181 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1472 | N | GLY | 2 | 688 | 26.544 | 54.866 | 34.851 | 1.00 | 0.00 |
| ATOM | 1473 | CA | GLY | 2 | 688 | 27.773 | 55.382 | 35.434 | 1.00 | 0.00 |
| ATOM | 1474 | C | GLY | 2 | 688 | 28.324 | 54.573 | 36.595 | 1.00 | 0.00 |
| ATOM | 1475 | O | GLY | 2 | 688 | 28.514 | 55.020 | 37.730 | 1.00 | 0.00 |
| ATOM | 1476 | H | GLY | 2 | 688 | 25.680 | 55.215 | 35.192 | 1.00 | 0.00 |
| ATOM | 1477 | N | ALA | 2 | 689 | 28.701 | 53.328 | 36.234 | 1.00 | 0.00 |
| ATOM | 1478 | CA | ALA | 2 | 689 | 29.587 | 52.607 | 37.152 | 1.00 | 0.00 |
| ATOM | 1479 | C | ALA | 2 | 689 | 30.813 | 53.458 | 37.462 | 1.00 | 0.00 |
| ATOM | 1480 | O | ALA | 2 | 689 | 30.929 | 54.029 | 38.549 | 1.00 | 0.00 |
| ATOM | 1481 | CB | ALA | 2 | 689 | 29.993 | 51.249 | 36.571 | 1.00 | 0.00 |
| ATOM | 1482 | H | ALA | 2 | 689 | 28.430 | 53.018 | 35.322 | 1.00 | 0.00 |
| ATOM | 1483 | N | THR | 2 | 690 | 31.620 | 53.627 | 36.391 | 1.00 | 0.00 |
| ATOM | 1484 | CA | THR | 2 | 690 | 32.630 | 54.686 | 36.354 | 1.00 | 0.00 |
| ATOM | 1485 | C | THR | 2 | 690 | 32.268 | 55.927 | 37.159 | 1.00 | 0.00 |
| ATOM | 1486 | O | THR | 2 | 690 | 32.825 | 56.139 | 38.234 | 1.00 | 0.00 |
| ATOM | 1487 | CB | THR | 2 | 690 | 32.930 | 55.031 | 34.895 | 1.00 | 0.00 |
| ATOM | 1488 | OG1 | THR | 2 | 690 | 31.709 | 55.049 | 34.132 | 1.00 | 0.00 |
| ATOM | 1489 | CG2 | THR | 2 | 690 | 33.923 | 54.047 | 34.273 | 1.00 | 0.00 |
| ATOM | 1490 | H | THR | 2 | 690 | 31.523 | 53.058 | 35.577 | 1.00 | 0.00 |
| ATOM | 1491 | HG1 | THR | 2 | 690 | 31.959 | 55.369 | 33.266 | 1.00 | 0.00 |
| ATOM | 1492 | N | MET | 2 | 691 | 31.251 | 56.655 | 36.653 | 1.00 | 0.00 |
| ATOM | 1493 | CA | MET | 2 | 691 | 30.851 | 57.935 | 37.256 | 1.00 | 0.00 |
| ATOM | 1494 | C | MET | 2 | 691 | 30.626 | 57.935 | 38.761 | 1.00 | 0.00 |
| ATOM | 1495 | O | MET | 2 | 691 | 31.390 | 58.479 | 39.565 | 1.00 | 0.00 |
| ATOM | 1496 | CB | MET | 2 | 691 | 29.598 | 58.505 | 36.577 | 1.00 | 0.00 |
| ATOM | 1497 | CG | MET | 2 | 691 | 29.625 | 58.614 | 35.051 | 1.00 | 0.00 |
| ATOM | 1498 | SD | MET | 2 | 691 | 28.003 | 59.100 | 34.428 | 1.00 | 0.00 |
| ATOM | 1499 | CE | MET | 2 | 691 | 28.079 | 58.266 | 32.833 | 1.00 | 0.00 |
| ATOM | 1500 | H | MET | 2 | 691 | 30.883 | 56.310 | 35.788 | 1.00 | 0.00 |
| ATOM | 1501 | N | THR | 2 | 692 | 29.506 | 57.302 | 39.148 | 1.00 | 0.00 |
| ATOM | 1502 | CA | THR | 2 | 692 | 29.107 | 57.441 | 40.549 | 1.00 | 0.00 |
| ATOM | 1503 | C | THR | 2 | 692 | 29.981 | 56.696 | 41.529 | 1.00 | 0.00 |
| ATOM | 1504 | O | THR | 2 | 692 | 29.821 | 56.818 | 42.742 | 1.00 | 0.00 |
| ATOM | 1505 | CB | THR | 2 | 692 | 27.643 | 57.033 | 40.755 | 1.00 | 0.00 |
| ATOM | 1506 | OG1 | THR | 2 | 692 | 27.130 | 57.503 | 42.024 | 1.00 | 0.00 |
| ATOM | 1507 | CG2 | THR | 2 | 692 | 27.452 | 55.521 | 40.586 | 1.00 | 0.00 |
| ATOM | 1508 | H | THR | 2 | 692 | 28.986 | 56.739 | 38.503 | 1.00 | 0.00 |
| ATOM | 1509 | HG1 | THR | 2 | 692 | 26.977 | 58.439 | 41.883 | 1.00 | 0.00 |
| ATOM | 1510 | N | PHE | 2 | 693 | 30.881 | 55.852 | 40.989 | 1.00 | 0.00 |
| ATOM | 1511 | CA | PHE | 2 | 693 | 31.826 | 55.316 | 41.959 | 1.00 | 0.00 |
| ATOM | 1512 | C | PHE | 2 | 693 | 33.073 | 56.159 | 42.109 | 1.00 | 0.00 |
| ATOM | 1513 | O | PHE | 2 | 693 | 33.580 | 56.336 | 43.215 | 1.00 | 0.00 |
| ATOM | 1514 | CB | PHE | 2 | 693 | 32.106 | 53.832 | 41.709 | 1.00 | 0.00 |
| ATOM | 1515 | CG | PHE | 2 | 693 | 30.840 | 53.049 | 41.992 | 1.00 | 0.00 |
| ATOM | 1516 | CD1 | PHE | 2 | 693 | 30.173 | 52.396 | 40.933 | 1.00 | 0.00 |
| ATOM | 1517 | CD2 | PHE | 2 | 693 | 30.334 | 52.996 | 43.310 | 1.00 | 0.00 |
| ATOM | 1518 | CE1 | PHE | 2 | 693 | 28.972 | 51.705 | 41.186 | 1.00 | 0.00 |
| ATOM | 1519 | CE2 | PHE | 2 | 693 | 29.133 | 52.306 | 43.568 | 1.00 | 0.00 |
| ATOM | 1520 | CZ | PHE | 2 | 693 | 28.459 | 51.676 | 42.500 | 1.00 | 0.00 |
| ATOM | 1521 | H | PHE | 2 | 693 | 30.981 | 55.720 | 39.999 | 1.00 | 0.00 |
| ATOM | 1522 | N | PHE | 2 | 694 | 33.495 | 56.711 | 40.950 | 1.00 | 0.00 |
| ATOM | 1523 | CA | PHE | 2 | 694 | 34.725 | 57.502 | 40.935 | 1.00 | 0.00 |
| ATOM | 1524 | C | PHE | 2 | 694 | 34.577 | 58.829 | 41.649 | 1.00 | 0.00 |
| ATOM | 1525 | O | PHE | 2 | 694 | 35.347 | 59.171 | 42.535 | 1.00 | 0.00 |
| ATOM | 1526 | CB | PHE | 2 | 694 | 35.215 | 57.687 | 39.493 | 1.00 | 0.00 |
| ATOM | 1527 | CG | PHE | 2 | 694 | 36.558 | 58.379 | 39.429 | 1.00 | 0.00 |
| ATOM | 1528 | CD1 | PHE | 2 | 694 | 36.627 | 59.686 | 38.901 | 1.00 | 0.00 |
| ATOM | 1529 | CD2 | PHE | 2 | 694 | 37.715 | 57.713 | 39.890 | 1.00 | 0.00 |
| ATOM | 1530 | CE1 | PHE | 2 | 694 | 37.873 | 60.340 | 38.832 | 1.00 | 0.00 |
| ATOM | 1531 | CE2 | PHE | 2 | 694 | 38.961 | 58.365 | 39.822 | 1.00 | 0.00 |
| ATOM | 1532 | CZ | PHE | 2 | 694 | 39.027 | 59.672 | 39.294 | 1.00 | 0.00 |
| ATOM | 1533 | H | PHE | 2 | 694 | 33.005 | 56.602 | 40.087 | 1.00 | 0.00 |
| ATOM | 1534 | N | LYS | 2 | 695 | 33.510 | 59.551 | 41.264 | 1.00 | 0.00 |
| ATOM | 1535 | CA | LYS | 2 | 695 | 33.136 | 60.711 | 42.077 | 1.00 | 0.00 |
| ATOM | 1536 | C | LYS | 2 | 695 | 32.893 | 60.357 | 43.537 | 1.00 | 0.00 |
| ATOM | 1537 | O | LYS | 2 | 695 | 33.281 | 61.099 | 44.440 | 1.00 | 0.00 |
| ATOM | 1538 | CB | LYS | 2 | 695 | 31.913 | 61.426 | 41.491 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1539 | CG | LYS | 2 | 695 | 32.170 | 62.649 | 40.597 | 1.00 | 0.00 |
| ATOM | 1540 | CD | LYS | 2 | 695 | 32.771 | 63.884 | 41.294 | 1.00 | 0.00 |
| ATOM | 1541 | CE | LYS | 2 | 695 | 32.697 | 65.120 | 40.381 | 1.00 | 0.00 |
| ATOM | 1542 | NZ | LYS | 2 | 695 | 33.463 | 66.267 | 40.892 | 1.00 | 0.00 |
| ATOM | 1543 | H | LYS | 2 | 695 | 32.910 | 59.238 | 40.531 | 1.00 | 0.00 |
| ATOM | 1544 | 1HZ | LYS | 2 | 695 | 33.543 | 66.958 | 40.122 | 1.00 | 0.00 |
| ATOM | 1545 | 2HZ | LYS | 2 | 695 | 33.000 | 66.731 | 41.707 | 1.00 | 0.00 |
| ATOM | 1546 | 3HZ | LYS | 2 | 695 | 34.429 | 65.964 | 41.125 | 1.00 | 0.00 |
| ATOM | 1547 | N | LYS | 2 | 696 | 32.286 | 59.165 | 43.731 | 1.00 | 0.00 |
| ATOM | 1548 | CA | LYS | 2 | 696 | 32.174 | 58.647 | 45.093 | 1.00 | 0.00 |
| ATOM | 1549 | C | LYS | 2 | 696 | 33.478 | 58.576 | 45.859 | 1.00 | 0.00 |
| ATOM | 1550 | O | LYS | 2 | 696 | 33.491 | 58.920 | 47.030 | 1.00 | 0.00 |
| ATOM | 1551 | CB | LYS | 2 | 696 | 31.436 | 57.311 | 45.144 | 1.00 | 0.00 |
| ATOM | 1552 | CG | LYS | 2 | 696 | 31.097 | 56.740 | 46.520 | 1.00 | 0.00 |
| ATOM | 1553 | CD | LYS | 2 | 696 | 30.338 | 55.408 | 46.464 | 1.00 | 0.00 |
| ATOM | 1554 | CE | LYS | 2 | 696 | 28.852 | 55.500 | 46.085 | 1.00 | 0.00 |
| ATOM | 1555 | NZ | LYS | 2 | 696 | 28.631 | 55.769 | 44.662 | 1.00 | 0.00 |
| ATOM | 1556 | H | LYS | 2 | 696 | 31.939 | 58.697 | 42.920 | 1.00 | 0.00 |
| ATOM | 1557 | 1HZ | LYS | 2 | 696 | 29.139 | 56.611 | 44.318 | 1.00 | 0.00 |
| ATOM | 1558 | 2HZ | LYS | 2 | 696 | 28.941 | 54.980 | 44.073 | 1.00 | 0.00 |
| ATOM | 1559 | 3HZ | LYS | 2 | 696 | 27.613 | 55.898 | 44.508 | 1.00 | 0.00 |
| ATOM | 1560 | N | SER | 2 | 697 | 34.576 | 58.207 | 45.174 | 1.00 | 0.00 |
| ATOM | 1561 | CA | SER | 2 | 697 | 35.897 | 58.185 | 45.827 | 1.00 | 0.00 |
| ATOM | 1562 | C | SER | 2 | 697 | 36.302 | 59.436 | 46.622 | 1.00 | 0.00 |
| ATOM | 1563 | O | SER | 2 | 697 | 37.083 | 59.404 | 47.570 | 1.00 | 0.00 |
| ATOM | 1564 | CB | SER | 2 | 697 | 36.985 | 57.824 | 44.811 | 1.00 | 0.00 |
| ATOM | 1565 | OG | SER | 2 | 697 | 36.514 | 56.831 | 43.871 | 1.00 | 0.00 |
| ATOM | 1566 | H | SER | 2 | 697 | 34.467 | 57.841 | 44.249 | 1.00 | 0.00 |
| ATOM | 1567 | HG | SER | 2 | 697 | 36.132 | 57.339 | 43.152 | 1.00 | 0.00 |
| ATOM | 1568 | N | LYS | 2 | 698 | 35.666 | 60.556 | 46.231 | 1.00 | 0.00 |
| ATOM | 1569 | CA | LYS | 2 | 698 | 35.780 | 61.775 | 47.024 | 1.00 | 0.00 |
| ATOM | 1570 | C | LYS | 2 | 698 | 35.464 | 61.608 | 48.509 | 1.00 | 0.00 |
| ATOM | 1571 | O | LYS | 2 | 698 | 36.235 | 62.055 | 49.349 | 1.00 | 0.00 |
| ATOM | 1572 | CB | LYS | 2 | 698 | 35.031 | 62.922 | 46.336 | 1.00 | 0.00 |
| ATOM | 1573 | CG | LYS | 2 | 698 | 35.640 | 64.297 | 46.616 | 1.00 | 0.00 |
| ATOM | 1574 | CD | LYS | 2 | 698 | 35.141 | 65.387 | 45.660 | 1.00 | 0.00 |
| ATOM | 1575 | CE | LYS | 2 | 698 | 35.556 | 66.799 | 46.095 | 1.00 | 0.00 |
| ATOM | 1576 | NZ | LYS | 2 | 698 | 34.768 | 67.173 | 47.272 | 1.00 | 0.00 |
| ATOM | 1577 | H | LYS | 2 | 698 | 35.141 | 60.522 | 45.384 | 1.00 | 0.00 |
| ATOM | 1578 | 1HZ | LYS | 2 | 698 | 33.776 | 67.373 | 47.041 | 1.00 | 0.00 |
| ATOM | 1579 | 2HZ | LYS | 2 | 698 | 34.752 | 66.390 | 47.955 | 1.00 | 0.00 |
| ATOM | 1580 | 3HZ | LYS | 2 | 698 | 35.143 | 67.994 | 47.779 | 1.00 | 0.00 |
| ATOM | 1581 | N | ILE | 2 | 699 | 34.400 | 60.848 | 48.828 | 1.00 | 0.00 |
| ATOM | 1582 | CA | ILE | 2 | 699 | 34.267 | 60.455 | 50.239 | 1.00 | 0.00 |
| ATOM | 1583 | C | ILE | 2 | 699 | 35.421 | 59.618 | 50.798 | 1.00 | 0.00 |
| ATOM | 1584 | O | ILE | 2 | 699 | 35.839 | 59.740 | 51.943 | 1.00 | 0.00 |
| ATOM | 1585 | CB | ILE | 2 | 699 | 32.893 | 59.811 | 50.541 | 1.00 | 0.00 |
| ATOM | 1586 | CG1 | ILE | 2 | 699 | 32.601 | 59.806 | 52.044 | 1.00 | 0.00 |
| ATOM | 1587 | CG2 | ILE | 2 | 699 | 32.764 | 58.385 | 49.985 | 1.00 | 0.00 |
| ATOM | 1588 | CD1 | ILE | 2 | 699 | 31.219 | 59.250 | 52.394 | 1.00 | 0.00 |
| ATOM | 1589 | H | ILE | 2 | 699 | 33.857 | 60.438 | 48.097 | 1.00 | 0.00 |
| ATOM | 1590 | N | SER | 2 | 700 | 35.968 | 58.748 | 49.943 | 1.00 | 0.00 |
| ATOM | 1591 | CA | SER | 2 | 700 | 37.015 | 57.846 | 50.434 | 1.00 | 0.00 |
| ATOM | 1592 | C | SER | 2 | 700 | 38.337 | 58.511 | 50.826 | 1.00 | 0.00 |
| ATOM | 1593 | O | SER | 2 | 700 | 38.984 | 58.158 | 51.805 | 1.00 | 0.00 |
| ATOM | 1594 | CB | SER | 2 | 700 | 37.187 | 56.713 | 49.423 | 1.00 | 0.00 |
| ATOM | 1595 | OG | SER | 2 | 700 | 35.890 | 56.191 | 49.087 | 1.00 | 0.00 |
| ATOM | 1596 | H | SER | 2 | 700 | 35.672 | 58.682 | 48.988 | 1.00 | 0.00 |
| ATOM | 1597 | HG | SER | 2 | 700 | 35.948 | 55.265 | 49.307 | 1.00 | 0.00 |
| ATOM | 1598 | N | THR | 2 | 701 | 38.675 | 59.545 | 50.042 | 1.00 | 0.00 |
| ATOM | 1599 | CA | THR | 2 | 701 | 39.640 | 60.508 | 50.566 | 1.00 | 0.00 |
| ATOM | 1600 | C | THR | 2 | 701 | 38.903 | 61.717 | 51.116 | 1.00 | 0.00 |
| ATOM | 1601 | O | THR | 2 | 701 | 38.621 | 62.686 | 50.420 | 1.00 | 0.00 |
| ATOM | 1602 | CB | THR | 2 | 701 | 40.652 | 60.892 | 49.483 | 1.00 | 0.00 |
| ATOM | 1603 | OG1 | THR | 2 | 701 | 41.247 | 59.709 | 48.931 | 1.00 | 0.00 |
| ATOM | 1604 | CG2 | THR | 2 | 701 | 41.749 | 61.827 | 50.006 | 1.00 | 0.00 |
| ATOM | 1605 | H | THR | 2 | 701 | 38.194 | 59.742 | 49.186 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1606 | HG1 | THR | 2 | 701 | 41.834 | 59.361 | 49.597 | 1.00 | 0.00 |
| ATOM | 1607 | N | TYR | 2 | 702 | 38.558 | 61.560 | 52.403 | 1.00 | 0.00 |
| ATOM | 1608 | CA | TYR | 2 | 702 | 37.478 | 62.310 | 53.060 | 1.00 | 0.00 |
| ATOM | 1609 | C | TYR | 2 | 702 | 37.190 | 63.788 | 52.821 | 1.00 | 0.00 |
| ATOM | 1610 | O | TYR | 2 | 702 | 37.393 | 64.633 | 53.689 | 1.00 | 0.00 |
| ATOM | 1611 | CB | TYR | 2 | 702 | 37.478 | 62.002 | 54.563 | 1.00 | 0.00 |
| ATOM | 1612 | CG | TYR | 2 | 702 | 36.868 | 60.636 | 54.741 | 1.00 | 0.00 |
| ATOM | 1613 | CD1 | TYR | 2 | 702 | 37.698 | 59.497 | 54.696 | 1.00 | 0.00 |
| ATOM | 1614 | CD2 | TYR | 2 | 702 | 35.470 | 60.541 | 54.891 | 1.00 | 0.00 |
| ATOM | 1615 | CE1 | TYR | 2 | 702 | 37.102 | 58.228 | 54.673 | 1.00 | 0.00 |
| ATOM | 1616 | CE2 | TYR | 2 | 702 | 34.875 | 59.271 | 54.872 | 1.00 | 0.00 |
| ATOM | 1617 | CZ | TYR | 2 | 702 | 35.697 | 58.139 | 54.710 | 1.00 | 0.00 |
| ATOM | 1618 | OH | TYR | 2 | 702 | 35.099 | 56.907 | 54.559 | 1.00 | 0.00 |
| ATOM | 1619 | H | TYR | 2 | 702 | 38.925 | 60.744 | 52.853 | 1.00 | 0.00 |
| ATOM | 1620 | HH | TYR | 2 | 702 | 35.731 | 56.250 | 54.834 | 1.00 | 0.00 |
| ATOM | 1621 | N | ASP | 2 | 703 | 36.579 | 64.027 | 51.648 | 1.00 | 0.00 |
| ATOM | 1622 | CA | ASP | 2 | 703 | 35.448 | 64.963 | 51.588 | 1.00 | 0.00 |
| ATOM | 1623 | C | ASP | 2 | 703 | 34.256 | 64.207 | 52.137 | 1.00 | 0.00 |
| ATOM | 1624 | O | ASP | 2 | 703 | 34.231 | 62.982 | 52.066 | 1.00 | 0.00 |
| ATOM | 1625 | CB | ASP | 2 | 703 | 35.219 | 65.378 | 50.121 | 1.00 | 0.00 |
| ATOM | 1626 | CG | ASP | 2 | 703 | 33.832 | 65.948 | 49.788 | 1.00 | 0.00 |
| ATOM | 1627 | OD1 | ASP | 2 | 703 | 33.269 | 66.703 | 50.565 | 1.00 | 0.00 |
| ATOM | 1628 | OD2 | ASP | 2 | 703 | 33.304 | 65.647 | 48.721 | 1.00 | 0.00 |
| ATOM | 1629 | H | ASP | 2 | 703 | 36.707 | 63.348 | 50.924 | 1.00 | 0.00 |
| ATOM | 1630 | N | LYS | 2 | 704 | 33.284 | 64.936 | 52.692 | 1.00 | 0.00 |
| ATOM | 1631 | CA | LYS | 2 | 704 | 32.109 | 64.199 | 53.137 | 1.00 | 0.00 |
| ATOM | 1632 | C | LYS | 2 | 704 | 31.292 | 63.620 | 51.980 | 1.00 | 0.00 |
| ATOM | 1633 | O | LYS | 2 | 704 | 30.785 | 62.506 | 52.050 | 1.00 | 0.00 |
| ATOM | 1634 | CB | LYS | 2 | 704 | 31.329 | 65.089 | 54.117 | 1.00 | 0.00 |
| ATOM | 1635 | CG | LYS | 2 | 704 | 30.131 | 64.468 | 54.848 | 1.00 | 0.00 |
| ATOM | 1636 | CD | LYS | 2 | 704 | 28.823 | 64.667 | 54.084 | 1.00 | 0.00 |
| ATOM | 1637 | CE | LYS | 2 | 704 | 28.516 | 66.153 | 53.906 | 1.00 | 0.00 |
| ATOM | 1638 | NZ | LYS | 2 | 704 | 27.622 | 66.324 | 52.767 | 1.00 | 0.00 |
| ATOM | 1639 | H | LYS | 2 | 704 | 33.361 | 65.928 | 52.585 | 1.00 | 0.00 |
| ATOM | 1640 | 1HZ | LYS | 2 | 704 | 27.777 | 67.229 | 52.275 | 1.00 | 0.00 |
| ATOM | 1641 | 2HZ | LYS | 2 | 704 | 27.819 | 65.567 | 52.090 | 1.00 | 0.00 |
| ATOM | 1642 | 3HZ | LYS | 2 | 704 | 26.643 | 66.266 | 53.091 | 1.00 | 0.00 |
| ATOM | 1643 | N | MET | 2 | 705 | 31.189 | 64.432 | 50.914 | 1.00 | 0.00 |
| ATOM | 1644 | CA | MET | 2 | 705 | 30.542 | 64.032 | 49.655 | 1.00 | 0.00 |
| ATOM | 1645 | C | MET | 2 | 705 | 29.030 | 63.795 | 49.606 | 1.00 | 0.00 |
| ATOM | 1646 | O | MET | 2 | 705 | 28.391 | 63.984 | 48.571 | 1.00 | 0.00 |
| ATOM | 1647 | CB | MET | 2 | 705 | 31.298 | 62.880 | 48.992 | 1.00 | 0.00 |
| ATOM | 1648 | CG | MET | 2 | 705 | 31.066 | 62.787 | 47.487 | 1.00 | 0.00 |
| ATOM | 1649 | SD | MET | 2 | 705 | 31.326 | 61.114 | 46.916 | 1.00 | 0.00 |
| ATOM | 1650 | CE | MET | 2 | 705 | 30.137 | 60.314 | 48.004 | 1.00 | 0.00 |
| ATOM | 1651 | H | MET | 2 | 705 | 31.738 | 65.270 | 50.881 | 1.00 | 0.00 |
| ATOM | 1652 | N | TRP | 2 | 706 | 28.463 | 63.403 | 50.767 | 1.00 | 0.00 |
| ATOM | 1653 | CA | TRP | 2 | 706 | 27.033 | 63.150 | 50.992 | 1.00 | 0.00 |
| ATOM | 1654 | C | TRP | 2 | 706 | 26.531 | 61.856 | 50.380 | 1.00 | 0.00 |
| ATOM | 1655 | O | TRP | 2 | 706 | 26.956 | 61.431 | 49.309 | 1.00 | 0.00 |
| ATOM | 1656 | CB | TRP | 2 | 706 | 26.146 | 64.345 | 50.594 | 1.00 | 0.00 |
| ATOM | 1657 | CG | TRP | 2 | 706 | 24.916 | 64.431 | 51.472 | 1.00 | 0.00 |
| ATOM | 1658 | CD1 | TRP | 2 | 706 | 24.871 | 64.383 | 52.877 | 1.00 | 0.00 |
| ATOM | 1659 | CD2 | TRP | 2 | 706 | 23.543 | 64.600 | 51.058 | 1.00 | 0.00 |
| ATOM | 1660 | NE1 | TRP | 2 | 706 | 23.598 | 64.510 | 53.341 | 1.00 | 0.00 |
| ATOM | 1661 | CE2 | TRP | 2 | 706 | 22.743 | 64.646 | 52.250 | 1.00 | 0.00 |
| ATOM | 1662 | CE3 | TRP | 2 | 706 | 22.931 | 64.716 | 49.793 | 1.00 | 0.00 |
| ATOM | 1663 | CZ2 | TRP | 2 | 706 | 21.345 | 64.809 | 52.149 | 1.00 | 0.00 |
| ATOM | 1664 | CZ3 | TRP | 2 | 706 | 21.532 | 64.877 | 49.708 | 1.00 | 0.00 |
| ATOM | 1665 | CH2 | TRP | 2 | 706 | 20.743 | 64.924 | 50.878 | 1.00 | 0.00 |
| ATOM | 1666 | H | TRP | 2 | 706 | 29.126 | 63.077 | 51.439 | 1.00 | 0.00 |
| ATOM | 1667 | HE1 | TRP | 2 | 706 | 23.323 | 64.513 | 54.287 | 1.00 | 0.00 |
| ATOM | 1668 | N | ALA | 2 | 707 | 25.594 | 61.218 | 51.112 | 1.00 | 0.00 |
| ATOM | 1669 | CA | ALA | 2 | 707 | 24.936 | 60.065 | 50.492 | 1.00 | 0.00 |
| ATOM | 1670 | C | ALA | 2 | 707 | 24.117 | 60.520 | 49.301 | 1.00 | 0.00 |
| ATOM | 1671 | O | ALA | 2 | 707 | 23.422 | 61.531 | 49.382 | 1.00 | 0.00 |
| ATOM | 1672 | CB | ALA | 2 | 707 | 24.022 | 59.360 | 51.494 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1673 | H | ALA | 2 | 707 | 25.199 | 61.681 | 51.906 | 1.00 | 0.00 |
| ATOM | 1674 | N | PHE | 2 | 708 | 24.281 | 59.789 | 48.195 | 1.00 | 0.00 |
| ATOM | 1675 | CA | PHE | 2 | 708 | 23.842 | 60.323 | 46.909 | 1.00 | 0.00 |
| ATOM | 1676 | C | PHE | 2 | 708 | 23.476 | 59.232 | 45.913 | 1.00 | 0.00 |
| ATOM | 1677 | O | PHE | 2 | 708 | 23.516 | 58.033 | 46.207 | 1.00 | 0.00 |
| ATOM | 1678 | CB | PHE | 2 | 708 | 24.904 | 61.298 | 46.346 | 1.00 | 0.00 |
| ATOM | 1679 | CG | PHE | 2 | 708 | 26.047 | 60.590 | 45.643 | 1.00 | 0.00 |
| ATOM | 1680 | CD1 | PHE | 2 | 708 | 26.223 | 60.808 | 44.260 | 1.00 | 0.00 |
| ATOM | 1681 | CD2 | PHE | 2 | 708 | 26.902 | 59.721 | 46.356 | 1.00 | 0.00 |
| ATOM | 1682 | CE1 | PHE | 2 | 708 | 27.259 | 60.144 | 43.577 | 1.00 | 0.00 |
| ATOM | 1683 | CE2 | PHE | 2 | 708 | 27.936 | 59.054 | 45.673 | 1.00 | 0.00 |
| ATOM | 1684 | CZ | PHE | 2 | 708 | 28.107 | 59.274 | 44.291 | 1.00 | 0.00 |
| ATOM | 1685 | H | PHE | 2 | 708 | 24.801 | 58.939 | 48.225 | 1.00 | 0.00 |
| ATOM | 1686 | N | MET | 2 | 709 | 23.145 | 59.676 | 44.681 | 1.00 | 0.00 |
| ATOM | 1687 | CA | MET | 2 | 709 | 22.849 | 58.693 | 43.623 | 1.00 | 0.00 |
| ATOM | 1688 | C | MET | 2 | 709 | 23.980 | 57.725 | 43.342 | 1.00 | 0.00 |
| ATOM | 1689 | O | MET | 2 | 709 | 25.078 | 57.878 | 43.878 | 1.00 | 0.00 |
| ATOM | 1690 | CB | MET | 2 | 709 | 22.417 | 59.374 | 42.325 | 1.00 | 0.00 |
| ATOM | 1691 | CG | MET | 2 | 709 | 21.031 | 60.001 | 42.426 | 1.00 | 0.00 |
| ATOM | 1692 | SD | MET | 2 | 709 | 20.587 | 60.953 | 40.975 | 1.00 | 0.00 |
| ATOM | 1693 | CE | MET | 2 | 709 | 19.753 | 62.309 | 41.821 | 1.00 | 0.00 |
| ATOM | 1694 | H | MET | 2 | 709 | 22.986 | 60.660 | 44.585 | 1.00 | 0.00 |
| ATOM | 1695 | N | SER | 2 | 710 | 23.636 | 56.713 | 42.543 | 1.00 | 0.00 |
| ATOM | 1696 | CA | SER | 2 | 710 | 24.429 | 55.542 | 42.165 | 1.00 | 0.00 |
| ATOM | 1697 | C | SER | 2 | 710 | 23.439 | 54.677 | 41.431 | 1.00 | 0.00 |
| ATOM | 1698 | O | SER | 2 | 710 | 22.419 | 55.206 | 40.997 | 1.00 | 0.00 |
| ATOM | 1699 | CB | SER | 2 | 710 | 25.006 | 54.803 | 43.381 | 1.00 | 0.00 |
| ATOM | 1700 | OG | SER | 2 | 710 | 26.140 | 55.523 | 43.895 | 1.00 | 0.00 |
| ATOM | 1701 | H | SER | 2 | 710 | 22.760 | 56.797 | 42.070 | 1.00 | 0.00 |
| ATOM | 1702 | HG | SER | 2 | 710 | 26.128 | 56.357 | 43.406 | 1.00 | 0.00 |
| ATOM | 1703 | N | SER | 2 | 711 | 23.666 | 53.358 | 41.420 | 1.00 | 0.00 |
| ATOM | 1704 | CA | SER | 2 | 711 | 22.546 | 52.474 | 41.085 | 1.00 | 0.00 |
| ATOM | 1705 | C | SER | 2 | 711 | 21.407 | 52.431 | 42.110 | 1.00 | 0.00 |
| ATOM | 1706 | O | SER | 2 | 711 | 21.108 | 51.403 | 42.711 | 1.00 | 0.00 |
| ATOM | 1707 | CB | SER | 2 | 711 | 23.100 | 51.082 | 40.811 | 1.00 | 0.00 |
| ATOM | 1708 | OG | SER | 2 | 711 | 24.417 | 51.195 | 40.241 | 1.00 | 0.00 |
| ATOM | 1709 | H | SER | 2 | 711 | 24.580 | 52.983 | 41.580 | 1.00 | 0.00 |
| ATOM | 1710 | HG | SER | 2 | 711 | 24.286 | 51.393 | 39.309 | 1.00 | 0.00 |
| ATOM | 1711 | N | ARG | 2 | 712 | 20.803 | 53.617 | 42.308 | 1.00 | 0.00 |
| ATOM | 1712 | CA | ARG | 2 | 712 | 19.872 | 53.904 | 43.393 | 1.00 | 0.00 |
| ATOM | 1713 | C | ARG | 2 | 712 | 18.414 | 53.845 | 42.973 | 1.00 | 0.00 |
| ATOM | 1714 | O | ARG | 2 | 712 | 17.679 | 52.957 | 43.396 | 1.00 | 0.00 |
| ATOM | 1715 | CB | ARG | 2 | 712 | 20.193 | 55.272 | 44.036 | 1.00 | 0.00 |
| ATOM | 1716 | CG | ARG | 2 | 712 | 19.275 | 55.680 | 45.207 | 1.00 | 0.00 |
| ATOM | 1717 | CD | ARG | 2 | 712 | 19.446 | 57.136 | 45.664 | 1.00 | 0.00 |
| ATOM | 1718 | NE | ARG | 2 | 712 | 18.420 | 57.528 | 46.643 | 1.00 | 0.00 |
| ATOM | 1719 | CZ | ARG | 2 | 712 | 17.848 | 58.758 | 46.576 | 1.00 | 0.00 |
| ATOM | 1720 | NH1 | ARG | 2 | 712 | 16.902 | 59.114 | 47.439 | 1.00 | 0.00 |
| ATOM | 1721 | NH2 | ARG | 2 | 712 | 18.212 | 59.619 | 45.638 | 1.00 | 0.00 |
| ATOM | 1722 | H | ARG | 2 | 712 | 20.914 | 54.240 | 41.531 | 1.00 | 0.00 |
| ATOM | 1723 | HE | ARG | 2 | 712 | 18.245 | 56.916 | 47.424 | 1.00 | 0.00 |
| ATOM | 1724 | 1HH1 | ARG | 2 | 712 | 16.450 | 60.009 | 47.337 | 1.00 | 0.00 |
| ATOM | 1725 | 2HH1 | ARG | 2 | 712 | 16.606 | 58.527 | 48.194 | 1.00 | 0.00 |
| ATOM | 1726 | 1HH2 | ARG | 2 | 712 | 17.916 | 60.586 | 45.668 | 1.00 | 0.00 |
| ATOM | 1727 | 2HH2 | ARG | 2 | 712 | 18.864 | 59.400 | 44.905 | 1.00 | 0.00 |
| ATOM | 1728 | N | ARG | 2 | 713 | 18.000 | 54.879 | 42.202 | 1.00 | 0.00 |
| ATOM | 1729 | CA | ARG | 2 | 713 | 16.554 | 54.989 | 41.976 | 1.00 | 0.00 |
| ATOM | 1730 | C | ARG | 2 | 713 | 16.099 | 54.148 | 40.813 | 1.00 | 0.00 |
| ATOM | 1731 | O | ARG | 2 | 713 | 15.844 | 54.647 | 39.723 | 1.00 | 0.00 |
| ATOM | 1732 | CB | ARG | 2 | 713 | 16.089 | 56.436 | 41.770 | 1.00 | 0.00 |
| ATOM | 1733 | CG | ARG | 2 | 713 | 15.991 | 57.279 | 43.041 | 1.00 | 0.00 |
| ATOM | 1734 | CD | ARG | 2 | 713 | 15.538 | 58.720 | 42.772 | 1.00 | 0.00 |
| ATOM | 1735 | NE | ARG | 2 | 713 | 14.185 | 58.808 | 42.206 | 1.00 | 0.00 |
| ATOM | 1736 | CZ | ARG | 2 | 713 | 13.375 | 59.848 | 42.548 | 1.00 | 0.00 |
| ATOM | 1737 | NH1 | ARG | 2 | 713 | 12.131 | 59.910 | 42.078 | 1.00 | 0.00 |
| ATOM | 1738 | NH2 | ARG | 2 | 713 | 13.820 | 60.821 | 43.336 | 1.00 | 0.00 |
| ATOM | 1739 | H | ARG | 2 | 713 | 18.705 | 55.336 | 41.656 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1740 | HE | ARG | 2 | 713 | 13.902 | 58.167 | 41.481 | 1.00 | 0.00 |
| ATOM | 1741 | 1HH1 | ARG | 2 | 713 | 11.508 | 60.659 | 42.311 | 1.00 | 0.00 |
| ATOM | 1742 | 2HH1 | ARG | 2 | 713 | 11.786 | 59.194 | 41.463 | 1.00 | 0.00 |
| ATOM | 1743 | 1HH2 | ARG | 2 | 713 | 13.202 | 61.558 | 43.614 | 1.00 | 0.00 |
| ATOM | 1744 | 2HH2 | ARG | 2 | 713 | 14.778 | 60.823 | 43.629 | 1.00 | 0.00 |
| ATOM | 1745 | N | GLN | 2 | 714 | 16.033 | 52.858 | 41.115 | 1.00 | 0.00 |
| ATOM | 1746 | CA | GLN | 2 | 714 | 15.762 | 51.909 | 40.057 | 1.00 | 0.00 |
| ATOM | 1747 | C | GLN | 2 | 714 | 14.300 | 51.658 | 39.736 | 1.00 | 0.00 |
| ATOM | 1748 | O | GLN | 2 | 714 | 13.684 | 50.664 | 40.118 | 1.00 | 0.00 |
| ATOM | 1749 | CB | GLN | 2 | 714 | 16.598 | 50.637 | 40.270 | 1.00 | 0.00 |
| ATOM | 1750 | CG | GLN | 2 | 714 | 16.673 | 50.106 | 41.707 | 1.00 | 0.00 |
| ATOM | 1751 | CD | GLN | 2 | 714 | 15.380 | 49.426 | 42.097 | 1.00 | 0.00 |
| ATOM | 1752 | OE1 | GLN | 2 | 714 | 14.503 | 49.941 | 42.779 | 1.00 | 0.00 |
| ATOM | 1753 | NE2 | GLN | 2 | 714 | 15.288 | 48.173 | 41.651 | 1.00 | 0.00 |
| ATOM | 1754 | H | GLN | 2 | 714 | 16.150 | 52.592 | 42.072 | 1.00 | 0.00 |
| ATOM | 1755 | 1HE2 | GLN | 2 | 714 | 14.495 | 47.608 | 41.890 | 1.00 | 0.00 |
| ATOM | 1756 | 2HE2 | GLN | 2 | 714 | 16.007 | 47.798 | 41.063 | 1.00 | 0.00 |
| ATOM | 1757 | N | SER | 2 | 715 | 13.763 | 52.585 | 38.935 | 1.00 | 0.00 |
| ATOM | 1758 | CA | SER | 2 | 715 | 12.535 | 52.218 | 38.233 | 1.00 | 0.00 |
| ATOM | 1759 | C | SER | 2 | 715 | 12.744 | 51.316 | 37.013 | 1.00 | 0.00 |
| ATOM | 1760 | O | SER | 2 | 715 | 12.556 | 51.725 | 35.871 | 1.00 | 0.00 |
| ATOM | 1761 | CB | SER | 2 | 715 | 11.716 | 53.462 | 37.870 | 1.00 | 0.00 |
| ATOM | 1762 | OG | SER | 2 | 715 | 12.112 | 54.586 | 38.675 | 1.00 | 0.00 |
| ATOM | 1763 | H | SER | 2 | 715 | 14.267 | 53.428 | 38.747 | 1.00 | 0.00 |
| ATOM | 1764 | HG | SER | 2 | 715 | 12.869 | 54.938 | 38.202 | 1.00 | 0.00 |
| ATOM | 1765 | N | VAL | 2 | 716 | 13.098 | 50.063 | 37.348 | 1.00 | 0.00 |
| ATOM | 1766 | CA | VAL | 2 | 716 | 13.325 | 48.973 | 36.396 | 1.00 | 0.00 |
| ATOM | 1767 | C | VAL | 2 | 716 | 14.542 | 49.114 | 35.481 | 1.00 | 0.00 |
| ATOM | 1768 | O | VAL | 2 | 716 | 15.597 | 48.552 | 35.769 | 1.00 | 0.00 |
| ATOM | 1769 | CB | VAL | 2 | 716 | 12.039 | 48.575 | 35.633 | 1.00 | 0.00 |
| ATOM | 1770 | CG1 | VAL | 2 | 716 | 12.206 | 47.238 | 34.903 | 1.00 | 0.00 |
| ATOM | 1771 | CG2 | VAL | 2 | 716 | 10.827 | 48.505 | 36.569 | 1.00 | 0.00 |
| ATOM | 1772 | H | VAL | 2 | 716 | 13.338 | 49.918 | 38.306 | 1.00 | 0.00 |
| ATOM | 1773 | N | LEU | 2 | 717 | 14.341 | 49.817 | 34.360 | 1.00 | 0.00 |
| ATOM | 1774 | CA | LEU | 2 | 717 | 15.383 | 49.782 | 33.331 | 1.00 | 0.00 |
| ATOM | 1775 | C | LEU | 2 | 717 | 16.115 | 51.094 | 33.198 | 1.00 | 0.00 |
| ATOM | 1776 | O | LEU | 2 | 717 | 15.682 | 52.115 | 33.720 | 1.00 | 0.00 |
| ATOM | 1777 | CB | LEU | 2 | 717 | 14.796 | 49.387 | 31.974 | 1.00 | 0.00 |
| ATOM | 1778 | CG | LEU | 2 | 717 | 14.361 | 47.923 | 31.889 | 1.00 | 0.00 |
| ATOM | 1779 | CD1 | LEU | 2 | 717 | 13.643 | 47.626 | 30.572 | 1.00 | 0.00 |
| ATOM | 1780 | CD2 | LEU | 2 | 717 | 15.527 | 46.961 | 32.134 | 1.00 | 0.00 |
| ATOM | 1781 | H | LEU | 2 | 717 | 13.563 | 50.443 | 34.332 | 1.00 | 0.00 |
| ATOM | 1782 | N | VAL | 2 | 718 | 17.230 | 51.044 | 32.453 | 1.00 | 0.00 |
| ATOM | 1783 | CA | VAL | 2 | 718 | 18.124 | 52.185 | 32.183 | 1.00 | 0.00 |
| ATOM | 1784 | C | VAL | 2 | 718 | 17.494 | 53.580 | 32.265 | 1.00 | 0.00 |
| ATOM | 1785 | O | VAL | 2 | 718 | 17.775 | 54.374 | 33.169 | 1.00 | 0.00 |
| ATOM | 1786 | CB | VAL | 2 | 718 | 18.829 | 51.959 | 30.825 | 1.00 | 0.00 |
| ATOM | 1787 | CG1 | VAL | 2 | 718 | 19.740 | 53.116 | 30.397 | 1.00 | 0.00 |
| ATOM | 1788 | CG2 | VAL | 2 | 718 | 19.600 | 50.637 | 30.826 | 1.00 | 0.00 |
| ATOM | 1789 | H | VAL | 2 | 718 | 17.490 | 50.138 | 32.125 | 1.00 | 0.00 |
| ATOM | 1790 | N | LYS | 2 | 719 | 16.600 | 53.825 | 31.281 | 1.00 | 0.00 |
| ATOM | 1791 | CA | LYS | 2 | 719 | 15.978 | 55.143 | 31.127 | 1.00 | 0.00 |
| ATOM | 1792 | C | LYS | 2 | 719 | 15.116 | 55.591 | 32.298 | 1.00 | 0.00 |
| ATOM | 1793 | O | LYS | 2 | 719 | 14.860 | 56.769 | 32.528 | 1.00 | 0.00 |
| ATOM | 1794 | CB | LYS | 2 | 719 | 15.203 | 55.170 | 29.795 | 1.00 | 0.00 |
| ATOM | 1795 | CG | LYS | 2 | 719 | 14.316 | 56.399 | 29.533 | 1.00 | 0.00 |
| ATOM | 1796 | CD | LYS | 2 | 719 | 12.825 | 56.140 | 29.783 | 1.00 | 0.00 |
| ATOM | 1797 | CE | LYS | 2 | 719 | 12.097 | 57.278 | 30.510 | 1.00 | 0.00 |
| ATOM | 1798 | NZ | LYS | 2 | 719 | 12.287 | 57.178 | 31.961 | 1.00 | 0.00 |
| ATOM | 1799 | H | LYS | 2 | 719 | 16.459 | 53.094 | 30.614 | 1.00 | 0.00 |
| ATOM | 1800 | 1HZ | LYS | 2 | 719 | 11.773 | 57.930 | 32.457 | 1.00 | 0.00 |
| ATOM | 1801 | 2HZ | LYS | 2 | 719 | 11.899 | 56.285 | 32.320 | 1.00 | 0.00 |
| ATOM | 1802 | 3HZ | LYS | 2 | 719 | 13.279 | 57.230 | 32.264 | 1.00 | 0.00 |
| ATOM | 1803 | N | SER | 2 | 720 | 14.601 | 54.601 | 33.033 | 1.00 | 0.00 |
| ATOM | 1804 | CA | SER | 2 | 720 | 13.696 | 54.968 | 34.121 | 1.00 | 0.00 |
| ATOM | 1805 | C | SER | 2 | 720 | 14.274 | 54.812 | 35.514 | 1.00 | 0.00 |
| ATOM | 1806 | O | SER | 2 | 720 | 13.766 | 55.314 | 36.519 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1807 | CB | SER | 2 | 720 | 12.369 | 54.265 | 33.890 | 1.00 | 0.00 |
| ATOM | 1808 | OG | SER | 2 | 720 | 11.939 | 54.628 | 32.565 | 1.00 | 0.00 |
| ATOM | 1809 | H | SER | 2 | 720 | 14.854 | 53.650 | 32.852 | 1.00 | 0.00 |
| ATOM | 1810 | HG | SER | 2 | 720 | 11.261 | 53.994 | 32.333 | 1.00 | 0.00 |
| ATOM | 1811 | N | ASN | 2 | 721 | 15.456 | 54.181 | 35.491 | 1.00 | 0.00 |
| ATOM | 1812 | CA | ASN | 2 | 721 | 16.316 | 54.270 | 36.663 | 1.00 | 0.00 |
| ATOM | 1813 | C | ASN | 2 | 721 | 16.806 | 55.701 | 36.785 | 1.00 | 0.00 |
| ATOM | 1814 | O | ASN | 2 | 721 | 16.285 | 56.486 | 37.582 | 1.00 | 0.00 |
| ATOM | 1815 | CB | ASN | 2 | 721 | 17.423 | 53.194 | 36.601 | 1.00 | 0.00 |
| ATOM | 1816 | CG | ASN | 2 | 721 | 16.778 | 51.815 | 36.660 | 1.00 | 0.00 |
| ATOM | 1817 | OD1 | ASN | 2 | 721 | 15.625 | 51.687 | 37.050 | 1.00 | 0.00 |
| ATOM | 1818 | ND2 | ASN | 2 | 721 | 17.510 | 50.795 | 36.210 | 1.00 | 0.00 |
| ATOM | 1819 | H | ASN | 2 | 721 | 15.763 | 53.733 | 34.651 | 1.00 | 0.00 |
| ATOM | 1820 | 1HD2 | ASN | 2 | 721 | 17.063 | 49.893 | 36.173 | 1.00 | 0.00 |
| ATOM | 1821 | 2HD2 | ASN | 2 | 721 | 18.448 | 50.888 | 35.871 | 1.00 | 0.00 |
| ATOM | 1822 | N | GLU | 2 | 722 | 17.759 | 56.025 | 35.905 | 1.00 | 0.00 |
| ATOM | 1823 | CA | GLU | 2 | 722 | 18.148 | 57.403 | 35.625 | 1.00 | 0.00 |
| ATOM | 1824 | C | GLU | 2 | 722 | 17.061 | 58.480 | 35.773 | 1.00 | 0.00 |
| ATOM | 1825 | O | GLU | 2 | 722 | 17.243 | 59.481 | 36.476 | 1.00 | 0.00 |
| ATOM | 1826 | CB | GLU | 2 | 722 | 18.828 | 57.331 | 34.247 | 1.00 | 0.00 |
| ATOM | 1827 | CG | GLU | 2 | 722 | 19.229 | 58.604 | 33.495 | 1.00 | 0.00 |
| ATOM | 1828 | CD | GLU | 2 | 722 | 18.030 | 59.302 | 32.894 | 1.00 | 0.00 |
| ATOM | 1829 | OE1 | GLU | 2 | 722 | 17.051 | 58.635 | 32.577 | 1.00 | 0.00 |
| ATOM | 1830 | OE2 | GLU | 2 | 722 | 18.067 | 60.519 | 32.753 | 1.00 | 0.00 |
| ATOM | 1831 | H | GLU | 2 | 722 | 18.155 | 55.306 | 35.343 | 1.00 | 0.00 |
| ATOM | 1832 | N | GLU | 2 | 723 | 15.909 | 58.251 | 35.103 | 1.00 | 0.00 |
| ATOM | 1833 | CA | GLU | 2 | 723 | 14.983 | 59.315 | 34.671 | 1.00 | 0.00 |
| ATOM | 1834 | C | GLU | 2 | 723 | 15.211 | 60.748 | 35.128 | 1.00 | 0.00 |
| ATOM | 1835 | O | GLU | 2 | 723 | 14.765 | 61.190 | 36.190 | 1.00 | 0.00 |
| ATOM | 1836 | CB | GLU | 2 | 723 | 13.516 | 58.888 | 34.817 | 1.00 | 0.00 |
| ATOM | 1837 | CG | GLU | 2 | 723 | 12.525 | 59.781 | 34.037 | 1.00 | 0.00 |
| ATOM | 1838 | CD | GLU | 2 | 723 | 11.149 | 59.134 | 33.883 | 1.00 | 0.00 |
| ATOM | 1839 | OE1 | GLU | 2 | 723 | 11.006 | 57.952 | 34.176 | 1.00 | 0.00 |
| ATOM | 1840 | OE2 | GLU | 2 | 723 | 10.217 | 59.781 | 33.411 | 1.00 | 0.00 |
| ATOM | 1841 | H | GLU | 2 | 723 | 15.847 | 57.345 | 34.696 | 1.00 | 0.00 |
| ATOM | 1842 | N | GLY | 2 | 724 | 15.897 | 61.486 | 34.249 | 1.00 | 0.00 |
| ATOM | 1843 | CA | GLY | 2 | 724 | 16.315 | 62.875 | 34.483 | 1.00 | 0.00 |
| ATOM | 1844 | C | GLY | 2 | 724 | 15.229 | 63.938 | 34.365 | 1.00 | 0.00 |
| ATOM | 1845 | O | GLY | 2 | 724 | 15.289 | 64.893 | 33.591 | 1.00 | 0.00 |
| ATOM | 1846 | H | GLY | 2 | 724 | 16.286 | 60.937 | 33.503 | 1.00 | 0.00 |
| ATOM | 1847 | N | ILE | 2 | 725 | 14.201 | 63.692 | 35.190 | 1.00 | 0.00 |
| ATOM | 1848 | CA | ILE | 2 | 725 | 13.028 | 64.533 | 35.421 | 1.00 | 0.00 |
| ATOM | 1849 | C | ILE | 2 | 725 | 12.272 | 64.001 | 36.636 | 1.00 | 0.00 |
| ATOM | 1850 | O | ILE | 2 | 725 | 11.971 | 64.724 | 37.578 | 1.00 | 0.00 |
| ATOM | 1851 | CB | ILE | 2 | 725 | 12.139 | 64.708 | 34.166 | 1.00 | 0.00 |
| ATOM | 1852 | CG1 | ILE | 2 | 725 | 10.879 | 65.526 | 34.476 | 1.00 | 0.00 |
| ATOM | 1853 | CG2 | ILE | 2 | 725 | 11.773 | 63.376 | 33.498 | 1.00 | 0.00 |
| ATOM | 1854 | CD1 | ILE | 2 | 725 | 10.050 | 65.867 | 33.237 | 1.00 | 0.00 |
| ATOM | 1855 | H | ILE | 2 | 725 | 14.356 | 62.943 | 35.828 | 1.00 | 0.00 |
| ATOM | 1856 | N | GLN | 2 | 726 | 12.065 | 62.667 | 36.653 | 1.00 | 0.00 |
| ATOM | 1857 | CA | GLN | 2 | 726 | 11.506 | 62.025 | 37.851 | 1.00 | 0.00 |
| ATOM | 1858 | C | GLN | 2 | 726 | 12.336 | 62.322 | 39.100 | 1.00 | 0.00 |
| ATOM | 1859 | O | GLN | 2 | 726 | 11.862 | 62.703 | 40.173 | 1.00 | 0.00 |
| ATOM | 1860 | CB | GLN | 2 | 726 | 11.389 | 60.529 | 37.533 | 1.00 | 0.00 |
| ATOM | 1861 | CG | GLN | 2 | 726 | 10.910 | 59.559 | 38.615 | 1.00 | 0.00 |
| ATOM | 1862 | CD | GLN | 2 | 726 | 12.014 | 58.549 | 38.872 | 1.00 | 0.00 |
| ATOM | 1863 | OE1 | GLN | 2 | 726 | 12.623 | 58.521 | 39.938 | 1.00 | 0.00 |
| ATOM | 1864 | NE2 | GLN | 2 | 726 | 12.327 | 57.777 | 37.830 | 1.00 | 0.00 |
| ATOM | 1865 | H | GLN | 2 | 726 | 12.375 | 62.138 | 35.864 | 1.00 | 0.00 |
| ATOM | 1866 | 1HE2 | GLN | 2 | 726 | 13.137 | 57.187 | 37.852 | 1.00 | 0.00 |
| ATOM | 1867 | 2HE2 | GLN | 2 | 726 | 11.784 | 57.787 | 36.987 | 1.00 | 0.00 |
| ATOM | 1868 | N | ARG | 2 | 727 | 13.666 | 62.187 | 38.878 | 1.00 | 0.00 |
| ATOM | 1869 | CA | ARG | 2 | 727 | 14.569 | 62.634 | 39.941 | 1.00 | 0.00 |
| ATOM | 1870 | C | ARG | 2 | 727 | 14.462 | 64.140 | 40.208 | 1.00 | 0.00 |
| ATOM | 1871 | O | ARG | 2 | 727 | 13.927 | 64.564 | 41.228 | 1.00 | 0.00 |
| ATOM | 1872 | CB | ARG | 2 | 727 | 16.020 | 62.156 | 39.691 | 1.00 | 0.00 |
| ATOM | 1873 | CG | ARG | 2 | 727 | 16.160 | 60.626 | 39.551 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1874 | CD | ARG | 2 | 727 | 17.594 | 60.048 | 39.515 | 1.00 | 0.00 |
| ATOM | 1875 | NE | ARG | 2 | 727 | 17.547 | 58.600 | 39.272 | 1.00 | 0.00 |
| ATOM | 1876 | CZ | ARG | 2 | 727 | 18.563 | 57.711 | 39.345 | 1.00 | 0.00 |
| ATOM | 1877 | NH1 | ARG | 2 | 727 | 18.279 | 56.437 | 39.205 | 1.00 | 0.00 |
| ATOM | 1878 | NH2 | ARG | 2 | 727 | 19.829 | 58.046 | 39.543 | 1.00 | 0.00 |
| ATOM | 1879 | H | ARG | 2 | 727 | 14.013 | 61.920 | 37.975 | 1.00 | 0.00 |
| ATOM | 1880 | HE | ARG | 2 | 727 | 16.659 | 58.238 | 38.960 | 1.00 | 0.00 |
| ATOM | 1881 | 1HH1 | ARG | 2 | 727 | 19.002 | 55.734 | 39.262 | 1.00 | 0.00 |
| ATOM | 1882 | 2HH1 | ARG | 2 | 727 | 17.342 | 56.136 | 38.985 | 1.00 | 0.00 |
| ATOM | 1883 | 1HH2 | ARG | 2 | 727 | 20.521 | 57.306 | 39.498 | 1.00 | 0.00 |
| ATOM | 1884 | 2HH2 | ARG | 2 | 727 | 20.131 | 58.983 | 39.705 | 1.00 | 0.00 |
| ATOM | 1885 | N | VAL | 2 | 728 | 14.914 | 64.913 | 39.204 | 1.00 | 0.00 |
| ATOM | 1886 | CA | VAL | 2 | 728 | 15.109 | 66.361 | 39.398 | 1.00 | 0.00 |
| ATOM | 1887 | C | VAL | 2 | 728 | 13.907 | 67.154 | 39.927 | 1.00 | 0.00 |
| ATOM | 1888 | O | VAL | 2 | 728 | 14.000 | 68.030 | 40.793 | 1.00 | 0.00 |
| ATOM | 1889 | CB | VAL | 2 | 728 | 15.628 | 66.982 | 38.087 | 1.00 | 0.00 |
| ATOM | 1890 | CG1 | VAL | 2 | 728 | 15.968 | 68.464 | 38.248 | 1.00 | 0.00 |
| ATOM | 1891 | CG2 | VAL | 2 | 728 | 16.824 | 66.208 | 37.524 | 1.00 | 0.00 |
| ATOM | 1892 | H | VAL | 2 | 728 | 15.208 | 64.491 | 38.349 | 1.00 | 0.00 |
| ATOM | 1893 | N | LEU | 2 | 729 | 12.763 | 66.813 | 39.331 | 1.00 | 0.00 |
| ATOM | 1894 | CA | LEU | 2 | 729 | 11.544 | 67.557 | 39.633 | 1.00 | 0.00 |
| ATOM | 1895 | C | LEU | 2 | 729 | 10.735 | 66.977 | 40.773 | 1.00 | 0.00 |
| ATOM | 1896 | O | LEU | 2 | 729 | 9.604 | 67.372 | 41.053 | 1.00 | 0.00 |
| ATOM | 1897 | CB | LEU | 2 | 729 | 10.692 | 67.708 | 38.370 | 1.00 | 0.00 |
| ATOM | 1898 | CG | LEU | 2 | 729 | 10.761 | 69.099 | 37.728 | 1.00 | 0.00 |
| ATOM | 1899 | CD1 | LEU | 2 | 729 | 12.188 | 69.568 | 37.439 | 1.00 | 0.00 |
| ATOM | 1900 | CD2 | LEU | 2 | 729 | 9.883 | 69.172 | 36.478 | 1.00 | 0.00 |
| ATOM | 1901 | H | LEU | 2 | 729 | 12.717 | 66.033 | 38.714 | 1.00 | 0.00 |
| ATOM | 1902 | N | THR | 2 | 730 | 11.354 | 66.004 | 41.461 | 1.00 | 0.00 |
| ATOM | 1903 | CA | THR | 2 | 730 | 10.730 | 65.799 | 42.754 | 1.00 | 0.00 |
| ATOM | 1904 | C | THR | 2 | 730 | 11.425 | 66.568 | 43.852 | 1.00 | 0.00 |
| ATOM | 1905 | O | THR | 2 | 730 | 10.765 | 67.051 | 44.761 | 1.00 | 0.00 |
| ATOM | 1906 | CB | THR | 2 | 730 | 10.544 | 64.323 | 43.110 | 1.00 | 0.00 |
| ATOM | 1907 | OG1 | THR | 2 | 730 | 11.735 | 63.571 | 42.814 | 1.00 | 0.00 |
| ATOM | 1908 | CG2 | THR | 2 | 730 | 9.350 | 63.720 | 42.367 | 1.00 | 0.00 |
| ATOM | 1909 | H | THR | 2 | 730 | 12.291 | 65.752 | 41.231 | 1.00 | 0.00 |
| ATOM | 1910 | HG1 | THR | 2 | 730 | 11.643 | 63.291 | 41.899 | 1.00 | 0.00 |
| ATOM | 1911 | N | SER | 2 | 731 | 12.770 | 66.688 | 43.773 | 1.00 | 0.00 |
| ATOM | 1912 | CA | SER | 2 | 731 | 13.395 | 67.308 | 44.955 | 1.00 | 0.00 |
| ATOM | 1913 | C | SER | 2 | 731 | 14.793 | 67.903 | 44.842 | 1.00 | 0.00 |
| ATOM | 1914 | O | SER | 2 | 731 | 15.588 | 67.776 | 45.769 | 1.00 | 0.00 |
| ATOM | 1915 | CB | SER | 2 | 731 | 13.359 | 66.334 | 46.149 | 1.00 | 0.00 |
| ATOM | 1916 | OG | SER | 2 | 731 | 13.485 | 64.978 | 45.677 | 1.00 | 0.00 |
| ATOM | 1917 | H | SER | 2 | 731 | 13.294 | 66.366 | 42.980 | 1.00 | 0.00 |
| ATOM | 1918 | HG | SER | 2 | 731 | 12.718 | 64.555 | 46.067 | 1.00 | 0.00 |
| ATOM | 1919 | N | ASP | 2 | 732 | 15.096 | 68.533 | 43.686 | 1.00 | 0.00 |
| ATOM | 1920 | CA | ASP | 2 | 732 | 16.363 | 69.270 | 43.457 | 1.00 | 0.00 |
| ATOM | 1921 | C | ASP | 2 | 732 | 17.567 | 69.022 | 44.401 | 1.00 | 0.00 |
| ATOM | 1922 | O | ASP | 2 | 732 | 17.897 | 69.819 | 45.287 | 1.00 | 0.00 |
| ATOM | 1923 | CB | ASP | 2 | 732 | 16.047 | 70.765 | 43.249 | 1.00 | 0.00 |
| ATOM | 1924 | CG | ASP | 2 | 732 | 15.749 | 71.502 | 44.547 | 1.00 | 0.00 |
| ATOM | 1925 | OD1 | ASP | 2 | 732 | 16.311 | 72.575 | 44.758 | 1.00 | 0.00 |
| ATOM | 1926 | OD2 | ASP | 2 | 732 | 14.997 | 71.004 | 45.384 | 1.00 | 0.00 |
| ATOM | 1927 | H | ASP | 2 | 732 | 14.421 | 68.545 | 42.944 | 1.00 | 0.00 |
| ATOM | 1928 | N | TYR | 2 | 733 | 18.221 | 67.833 | 44.269 | 1.00 | 0.00 |
| ATOM | 1929 | CA | TYR | 2 | 733 | 18.285 | 66.865 | 43.151 | 1.00 | 0.00 |
| ATOM | 1930 | C | TYR | 2 | 733 | 18.880 | 67.408 | 41.867 | 1.00 | 0.00 |
| ATOM | 1931 | O | TYR | 2 | 733 | 18.205 | 67.881 | 40.953 | 1.00 | 0.00 |
| ATOM | 1932 | CB | TYR | 2 | 733 | 17.014 | 66.027 | 42.878 | 1.00 | 0.00 |
| ATOM | 1933 | CG | TYR | 2 | 733 | 16.822 | 64.878 | 43.852 | 1.00 | 0.00 |
| ATOM | 1934 | CD1 | TYR | 2 | 733 | 16.560 | 63.597 | 43.322 | 1.00 | 0.00 |
| ATOM | 1935 | CD2 | TYR | 2 | 733 | 16.886 | 65.095 | 45.244 | 1.00 | 0.00 |
| ATOM | 1936 | CE1 | TYR | 2 | 733 | 16.364 | 62.514 | 44.197 | 1.00 | 0.00 |
| ATOM | 1937 | CE2 | TYR | 2 | 733 | 16.683 | 64.016 | 46.120 | 1.00 | 0.00 |
| ATOM | 1938 | CZ | TYR | 2 | 733 | 16.439 | 62.732 | 45.587 | 1.00 | 0.00 |
| ATOM | 1939 | OH | TYR | 2 | 733 | 16.300 | 61.659 | 46.460 | 1.00 | 0.00 |
| ATOM | 1940 | H | TYR | 2 | 733 | 18.852 | 67.729 | 45.033 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1941 | HH | TYR | 2 | 733 | 16.619 | 61.979 | 47.309 | 1.00 | 0.00 |
| ATOM | 1942 | N | ALA | 2 | 734 | 20.218 | 67.306 | 41.907 | 1.00 | 0.00 |
| ATOM | 1943 | CA | ALA | 2 | 734 | 21.077 | 67.590 | 40.769 | 1.00 | 0.00 |
| ATOM | 1944 | C | ALA | 2 | 734 | 21.526 | 66.261 | 40.227 | 1.00 | 0.00 |
| ATOM | 1945 | O | ALA | 2 | 734 | 21.637 | 65.289 | 40.974 | 1.00 | 0.00 |
| ATOM | 1946 | CB | ALA | 2 | 734 | 22.323 | 68.340 | 41.231 | 1.00 | 0.00 |
| ATOM | 1947 | H | ALA | 2 | 734 | 20.603 | 66.800 | 42.673 | 1.00 | 0.00 |
| ATOM | 1948 | N | PHE | 2 | 735 | 21.785 | 66.235 | 38.924 | 1.00 | 0.00 |
| ATOM | 1949 | CA | PHE | 2 | 735 | 21.983 | 64.948 | 38.255 | 1.00 | 0.00 |
| ATOM | 1950 | C | PHE | 2 | 735 | 23.196 | 65.001 | 37.346 | 1.00 | 0.00 |
| ATOM | 1951 | O | PHE | 2 | 735 | 23.471 | 66.067 | 36.806 | 1.00 | 0.00 |
| ATOM | 1952 | CB | PHE | 2 | 735 | 20.686 | 64.637 | 37.501 | 1.00 | 0.00 |
| ATOM | 1953 | CG | PHE | 2 | 735 | 20.576 | 63.197 | 37.066 | 1.00 | 0.00 |
| ATOM | 1954 | CD1 | PHE | 2 | 735 | 20.179 | 62.924 | 35.740 | 1.00 | 0.00 |
| ATOM | 1955 | CD2 | PHE | 2 | 735 | 20.835 | 62.157 | 37.984 | 1.00 | 0.00 |
| ATOM | 1956 | CE1 | PHE | 2 | 735 | 20.007 | 61.589 | 35.336 | 1.00 | 0.00 |
| ATOM | 1957 | CE2 | PHE | 2 | 735 | 20.667 | 60.821 | 37.579 | 1.00 | 0.00 |
| ATOM | 1958 | CZ | PHE | 2 | 735 | 20.241 | 60.553 | 36.264 | 1.00 | 0.00 |
| ATOM | 1959 | H | PHE | 2 | 735 | 21.748 | 67.124 | 38.467 | 1.00 | 0.00 |
| ATOM | 1960 | N | LEU | 2 | 736 | 23.917 | 63.884 | 37.221 | 1.00 | 0.00 |
| ATOM | 1961 | CA | LEU | 2 | 736 | 25.170 | 63.983 | 36.474 | 1.00 | 0.00 |
| ATOM | 1962 | C | LEU | 2 | 736 | 25.212 | 63.021 | 35.306 | 1.00 | 0.00 |
| ATOM | 1963 | O | LEU | 2 | 736 | 24.709 | 61.897 | 35.394 | 1.00 | 0.00 |
| ATOM | 1964 | CB | LEU | 2 | 736 | 26.379 | 63.709 | 37.373 | 1.00 | 0.00 |
| ATOM | 1965 | CG | LEU | 2 | 736 | 26.969 | 64.904 | 38.129 | 1.00 | 0.00 |
| ATOM | 1966 | CD1 | LEU | 2 | 736 | 26.018 | 65.519 | 39.151 | 1.00 | 0.00 |
| ATOM | 1967 | CD2 | LEU | 2 | 736 | 28.295 | 64.534 | 38.789 | 1.00 | 0.00 |
| ATOM | 1968 | H | LEU | 2 | 736 | 23.651 | 63.035 | 37.662 | 1.00 | 0.00 |
| ATOM | 1969 | N | MET | 2 | 737 | 25.838 | 63.500 | 34.214 | 1.00 | 0.00 |
| ATOM | 1970 | CA | MET | 2 | 737 | 26.210 | 62.671 | 33.054 | 1.00 | 0.00 |
| ATOM | 1971 | C | MET | 2 | 737 | 27.184 | 63.399 | 32.118 | 1.00 | 0.00 |
| ATOM | 1972 | O | MET | 2 | 737 | 27.359 | 64.619 | 32.122 | 1.00 | 0.00 |
| ATOM | 1973 | CB | MET | 2 | 737 | 24.980 | 62.158 | 32.270 | 1.00 | 0.00 |
| ATOM | 1974 | CG | MET | 2 | 737 | 25.179 | 60.877 | 31.445 | 1.00 | 0.00 |
| ATOM | 1975 | SD | MET | 2 | 737 | 24.226 | 60.767 | 29.910 | 1.00 | 0.00 |
| ATOM | 1976 | CE | MET | 2 | 737 | 22.550 | 60.897 | 30.552 | 1.00 | 0.00 |
| ATOM | 1977 | H | MET | 2 | 737 | 26.069 | 64.478 | 34.197 | 1.00 | 0.00 |
| ATOM | 1978 | N | GLU | 2 | 738 | 27.863 | 62.582 | 31.307 | 1.00 | 0.00 |
| ATOM | 1979 | CA | GLU | 2 | 738 | 28.806 | 63.117 | 30.338 | 1.00 | 0.00 |
| ATOM | 1980 | C | GLU | 2 | 738 | 28.153 | 63.638 | 29.056 | 1.00 | 0.00 |
| ATOM | 1981 | O | GLU | 2 | 738 | 27.851 | 64.825 | 28.907 | 1.00 | 0.00 |
| ATOM | 1982 | CB | GLU | 2 | 738 | 29.903 | 62.067 | 30.117 | 1.00 | 0.00 |
| ATOM | 1983 | CG | GLU | 2 | 738 | 30.615 | 61.662 | 31.418 | 1.00 | 0.00 |
| ATOM | 1984 | CD | GLU | 2 | 738 | 31.354 | 60.340 | 31.264 | 1.00 | 0.00 |
| ATOM | 1985 | OE1 | GLU | 2 | 738 | 30.855 | 59.317 | 31.696 | 1.00 | 0.00 |
| ATOM | 1986 | OE2 | GLU | 2 | 738 | 32.430 | 60.286 | 30.697 | 1.00 | 0.00 |
| ATOM | 1987 | H | GLU | 2 | 738 | 27.597 | 61.625 | 31.323 | 1.00 | 0.00 |
| ATOM | 1988 | N | SER | 2 | 739 | 27.943 | 62.706 | 28.118 | 1.00 | 0.00 |
| ATOM | 1989 | CA | SER | 2 | 739 | 27.403 | 63.116 | 26.825 | 1.00 | 0.00 |
| ATOM | 1990 | C | SER | 2 | 739 | 25.943 | 63.550 | 26.853 | 1.00 | 0.00 |
| ATOM | 1991 | O | SER | 2 | 739 | 25.594 | 64.736 | 26.922 | 1.00 | 0.00 |
| ATOM | 1992 | CB | SER | 2 | 739 | 27.625 | 62.014 | 25.785 | 1.00 | 0.00 |
| ATOM | 1993 | OG | SER | 2 | 739 | 28.729 | 61.156 | 26.144 | 1.00 | 0.00 |
| ATOM | 1994 | H | SER | 2 | 739 | 28.181 | 61.749 | 28.262 | 1.00 | 0.00 |
| ATOM | 1995 | HG | SER | 2 | 739 | 29.161 | 60.908 | 25.325 | 1.00 | 0.00 |
| ATOM | 1996 | N | THR | 2 | 740 | 25.062 | 62.549 | 26.830 | 1.00 | 0.00 |
| ATOM | 1997 | CA | THR | 2 | 740 | 23.662 | 62.894 | 26.716 | 1.00 | 0.00 |
| ATOM | 1998 | C | THR | 2 | 740 | 22.988 | 63.536 | 27.918 | 1.00 | 0.00 |
| ATOM | 1999 | O | THR | 2 | 740 | 21.771 | 63.730 | 27.920 | 1.00 | 0.00 |
| ATOM | 2000 | CB | THR | 2 | 740 | 22.888 | 61.689 | 26.188 | 1.00 | 0.00 |
| ATOM | 2001 | OG1 | THR | 2 | 740 | 23.581 | 60.450 | 26.471 | 1.00 | 0.00 |
| ATOM | 2002 | CG2 | THR | 2 | 740 | 22.568 | 61.862 | 24.703 | 1.00 | 0.00 |
| ATOM | 2003 | H | THR | 2 | 740 | 25.357 | 61.611 | 26.683 | 1.00 | 0.00 |
| ATOM | 2004 | HG1 | THR | 2 | 740 | 23.522 | 60.384 | 27.426 | 1.00 | 0.00 |
| ATOM | 2005 | N | THR | 2 | 741 | 23.772 | 63.917 | 28.948 | 1.00 | 0.00 |
| ATOM | 2006 | CA | THR | 2 | 741 | 23.120 | 64.801 | 29.924 | 1.00 | 0.00 |
| ATOM | 2007 | C | THR | 2 | 741 | 22.608 | 66.102 | 29.346 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2008 | O | THR | 2 | 741 | 21.622 | 66.673 | 29.815 | 1.00 | 0.00 |
| ATOM | 2009 | CB | THR | 2 | 741 | 23.957 | 65.101 | 31.164 | 1.00 | 0.00 |
| ATOM | 2010 | OG1 | THR | 2 | 741 | 23.113 | 65.508 | 32.262 | 1.00 | 0.00 |
| ATOM | 2011 | CG2 | THR | 2 | 741 | 25.062 | 66.113 | 30.886 | 1.00 | 0.00 |
| ATOM | 2012 | H | THR | 2 | 741 | 24.717 | 63.587 | 29.019 | 1.00 | 0.00 |
| ATOM | 2013 | HG1 | THR | 2 | 741 | 22.789 | 66.381 | 32.047 | 1.00 | 0.00 |
| ATOM | 2014 | N | ILE | 2 | 742 | 23.294 | 66.543 | 28.276 | 1.00 | 0.00 |
| ATOM | 2015 | CA | ILE | 2 | 742 | 22.585 | 67.492 | 27.439 | 1.00 | 0.00 |
| ATOM | 2016 | C | ILE | 2 | 742 | 21.449 | 66.769 | 26.707 | 1.00 | 0.00 |
| ATOM | 2017 | O | ILE | 2 | 742 | 20.472 | 66.452 | 27.382 | 1.00 | 0.00 |
| ATOM | 2018 | CB | ILE | 2 | 742 | 23.576 | 68.377 | 26.649 | 1.00 | 0.00 |
| ATOM | 2019 | CG1 | ILE | 2 | 742 | 22.895 | 69.467 | 25.815 | 1.00 | 0.00 |
| ATOM | 2020 | CG2 | ILE | 2 | 742 | 24.599 | 67.559 | 25.845 | 1.00 | 0.00 |
| ATOM | 2021 | CD1 | ILE | 2 | 742 | 23.885 | 70.469 | 25.217 | 1.00 | 0.00 |
| ATOM | 2022 | H | ILE | 2 | 742 | 24.127 | 66.076 | 27.988 | 1.00 | 0.00 |
| ATOM | 2023 | N | GLU | 2 | 743 | 21.553 | 66.470 | 25.397 | 1.00 | 0.00 |
| ATOM | 2024 | CA | GLU | 2 | 743 | 20.388 | 65.938 | 24.666 | 1.00 | 0.00 |
| ATOM | 2025 | C | GLU | 2 | 743 | 19.367 | 65.096 | 25.435 | 1.00 | 0.00 |
| ATOM | 2026 | O | GLU | 2 | 743 | 18.205 | 65.475 | 25.589 | 1.00 | 0.00 |
| ATOM | 2027 | CB | GLU | 2 | 743 | 20.758 | 65.189 | 23.370 | 1.00 | 0.00 |
| ATOM | 2028 | CG | GLU | 2 | 743 | 22.028 | 65.570 | 22.592 | 1.00 | 0.00 |
| ATOM | 2029 | CD | GLU | 2 | 743 | 22.174 | 67.069 | 22.420 | 1.00 | 0.00 |
| ATOM | 2030 | OE1 | GLU | 2 | 743 | 21.469 | 67.690 | 21.632 | 1.00 | 0.00 |
| ATOM | 2031 | OE2 | GLU | 2 | 743 | 23.020 | 67.637 | 23.091 | 1.00 | 0.00 |
| ATOM | 2032 | H | GLU | 2 | 743 | 22.351 | 66.762 | 24.869 | 1.00 | 0.00 |
| ATOM | 2033 | N | PHE | 2 | 744 | 19.826 | 63.932 | 25.952 | 1.00 | 0.00 |
| ATOM | 2034 | CA | PHE | 2 | 744 | 18.873 | 63.053 | 26.654 | 1.00 | 0.00 |
| ATOM | 2035 | C | PHE | 2 | 744 | 18.194 | 63.689 | 27.860 | 1.00 | 0.00 |
| ATOM | 2036 | O | PHE | 2 | 744 | 16.974 | 63.703 | 28.005 | 1.00 | 0.00 |
| ATOM | 2037 | CB | PHE | 2 | 744 | 19.524 | 61.713 | 27.036 | 1.00 | 0.00 |
| ATOM | 2038 | CG | PHE | 2 | 744 | 18.532 | 60.701 | 27.566 | 1.00 | 0.00 |
| ATOM | 2039 | CD1 | PHE | 2 | 744 | 17.975 | 59.756 | 26.678 | 1.00 | 0.00 |
| ATOM | 2040 | CD2 | PHE | 2 | 744 | 18.183 | 60.712 | 28.935 | 1.00 | 0.00 |
| ATOM | 2041 | CE1 | PHE | 2 | 744 | 17.037 | 58.824 | 27.161 | 1.00 | 0.00 |
| ATOM | 2042 | CE2 | PHE | 2 | 744 | 17.245 | 59.781 | 29.419 | 1.00 | 0.00 |
| ATOM | 2043 | CZ | PHE | 2 | 744 | 16.677 | 58.852 | 28.524 | 1.00 | 0.00 |
| ATOM | 2044 | H | PHE | 2 | 744 | 20.816 | 63.780 | 25.949 | 1.00 | 0.00 |
| ATOM | 2045 | N | VAL | 2 | 745 | 19.023 | 64.255 | 28.739 | 1.00 | 0.00 |
| ATOM | 2046 | CA | VAL | 2 | 745 | 18.406 | 64.895 | 29.902 | 1.00 | 0.00 |
| ATOM | 2047 | C | VAL | 2 | 745 | 17.830 | 66.280 | 29.594 | 1.00 | 0.00 |
| ATOM | 2048 | O | VAL | 2 | 745 | 17.239 | 66.943 | 30.433 | 1.00 | 0.00 |
| ATOM | 2049 | CB | VAL | 2 | 745 | 19.381 | 64.871 | 31.102 | 1.00 | 0.00 |
| ATOM | 2050 | CG1 | VAL | 2 | 745 | 18.799 | 65.384 | 32.425 | 1.00 | 0.00 |
| ATOM | 2051 | CG2 | VAL | 2 | 745 | 19.896 | 63.446 | 31.308 | 1.00 | 0.00 |
| ATOM | 2052 | H | VAL | 2 | 745 | 20.008 | 64.255 | 28.573 | 1.00 | 0.00 |
| ATOM | 2053 | N | THR | 2 | 746 | 17.965 | 66.721 | 28.338 | 1.00 | 0.00 |
| ATOM | 2054 | CA | THR | 2 | 746 | 17.484 | 68.088 | 28.135 | 1.00 | 0.00 |
| ATOM | 2055 | C | THR | 2 | 746 | 16.289 | 68.254 | 27.201 | 1.00 | 0.00 |
| ATOM | 2056 | O | THR | 2 | 746 | 15.588 | 69.267 | 27.157 | 1.00 | 0.00 |
| ATOM | 2057 | CB | THR | 2 | 746 | 18.664 | 69.021 | 27.841 | 1.00 | 0.00 |
| ATOM | 2058 | OG1 | THR | 2 | 746 | 18.511 | 70.236 | 28.580 | 1.00 | 0.00 |
| ATOM | 2059 | CG2 | THR | 2 | 746 | 18.912 | 69.297 | 26.353 | 1.00 | 0.00 |
| ATOM | 2060 | H | THR | 2 | 746 | 18.415 | 66.193 | 27.617 | 1.00 | 0.00 |
| ATOM | 2061 | HG1 | THR | 2 | 746 | 18.091 | 70.008 | 29.415 | 1.00 | 0.00 |
| ATOM | 2062 | N | GLN | 2 | 747 | 16.042 | 67.136 | 26.501 | 1.00 | 0.00 |
| ATOM | 2063 | CA | GLN | 2 | 747 | 14.660 | 66.889 | 26.110 | 1.00 | 0.00 |
| ATOM | 2064 | C | GLN | 2 | 747 | 13.847 | 66.563 | 27.363 | 1.00 | 0.00 |
| ATOM | 2065 | O | GLN | 2 | 747 | 12.682 | 66.903 | 27.529 | 1.00 | 0.00 |
| ATOM | 2066 | CB | GLN | 2 | 747 | 14.657 | 65.735 | 25.108 | 1.00 | 0.00 |
| ATOM | 2067 | CG | GLN | 2 | 747 | 15.551 | 65.970 | 23.883 | 1.00 | 0.00 |
| ATOM | 2068 | CD | GLN | 2 | 747 | 16.083 | 64.649 | 23.344 | 1.00 | 0.00 |
| ATOM | 2069 | OE1 | GLN | 2 | 747 | 15.480 | 63.584 | 23.456 | 1.00 | 0.00 |
| ATOM | 2070 | NE2 | GLN | 2 | 747 | 17.269 | 64.751 | 22.751 | 1.00 | 0.00 |
| ATOM | 2071 | H | GLN | 2 | 747 | 16.693 | 66.379 | 26.556 | 1.00 | 0.00 |
| ATOM | 2072 | 1HE2 | GLN | 2 | 747 | 17.716 | 63.990 | 22.281 | 1.00 | 0.00 |
| ATOM | 2073 | 2HE2 | GLN | 2 | 747 | 17.739 | 65.635 | 22.771 | 1.00 | 0.00 |
| ATOM | 2074 | N | ARG | 2 | 748 | 14.564 | 65.901 | 28.288 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2075 | CA | ARG | 2 | 748 | 13.916 | 65.536 | 29.548 | 1.00 | 0.00 |
| ATOM | 2076 | C | ARG | 2 | 748 | 13.769 | 66.610 | 30.631 | 1.00 | 0.00 |
| ATOM | 2077 | O | ARG | 2 | 748 | 12.900 | 66.488 | 31.499 | 1.00 | 0.00 |
| ATOM | 2078 | CB | ARG | 2 | 748 | 14.532 | 64.241 | 30.093 | 1.00 | 0.00 |
| ATOM | 2079 | CG | ARG | 2 | 748 | 13.731 | 62.970 | 29.759 | 1.00 | 0.00 |
| ATOM | 2080 | CD | ARG | 2 | 748 | 13.480 | 62.667 | 28.271 | 1.00 | 0.00 |
| ATOM | 2081 | NE | ARG | 2 | 748 | 14.703 | 62.318 | 27.547 | 1.00 | 0.00 |
| ATOM | 2082 | CZ | ARG | 2 | 748 | 14.749 | 62.301 | 26.194 | 1.00 | 0.00 |
| ATOM | 2083 | NH1 | ARG | 2 | 748 | 15.865 | 61.942 | 25.582 | 1.00 | 0.00 |
| ATOM | 2084 | NH2 | ARG | 2 | 748 | 13.706 | 62.663 | 25.454 | 1.00 | 0.00 |
| ATOM | 2085 | H | ARG | 2 | 748 | 15.528 | 65.682 | 28.143 | 1.00 | 0.00 |
| ATOM | 2086 | HE | ARG | 2 | 748 | 15.537 | 62.117 | 28.073 | 1.00 | 0.00 |
| ATOM | 2087 | 1HH1 | ARG | 2 | 748 | 16.654 | 61.622 | 26.104 | 1.00 | 0.00 |
| ATOM | 2088 | 2HH1 | ARG | 2 | 748 | 15.943 | 61.981 | 24.582 | 1.00 | 0.00 |
| ATOM | 2089 | 1HH2 | ARG | 2 | 748 | 13.829 | 62.798 | 24.462 | 1.00 | 0.00 |
| ATOM | 2090 | 2HH2 | ARG | 2 | 748 | 12.800 | 62.832 | 25.844 | 1.00 | 0.00 |
| ATOM | 2091 | N | ASN | 2 | 749 | 14.582 | 67.690 | 30.551 | 1.00 | 0.00 |
| ATOM | 2092 | CA | ASN | 2 | 749 | 14.419 | 68.698 | 31.616 | 1.00 | 0.00 |
| ATOM | 2093 | C | ASN | 2 | 749 | 14.864 | 70.147 | 31.372 | 1.00 | 0.00 |
| ATOM | 2094 | O | ASN | 2 | 749 | 15.126 | 70.888 | 32.330 | 1.00 | 0.00 |
| ATOM | 2095 | CB | ASN | 2 | 749 | 15.013 | 68.174 | 32.941 | 1.00 | 0.00 |
| ATOM | 2096 | CG | ASN | 2 | 749 | 14.174 | 68.558 | 34.157 | 1.00 | 0.00 |
| ATOM | 2097 | OD1 | ASN | 2 | 749 | 14.684 | 68.984 | 35.189 | 1.00 | 0.00 |
| ATOM | 2098 | ND2 | ASN | 2 | 749 | 12.859 | 68.334 | 34.009 | 1.00 | 0.00 |
| ATOM | 2099 | H | ASN | 2 | 749 | 15.428 | 67.595 | 30.033 | 1.00 | 0.00 |
| ATOM | 2100 | 1HD2 | ASN | 2 | 749 | 12.213 | 68.537 | 34.744 | 1.00 | 0.00 |
| ATOM | 2101 | 2HD2 | ASN | 2 | 749 | 12.501 | 67.900 | 33.178 | 1.00 | 0.00 |
| ATOM | 2102 | N | CYS | 2 | 750 | 14.929 | 70.515 | 30.063 | 1.00 | 0.00 |
| ATOM | 2103 | CA | CYS | 2 | 750 | 15.353 | 71.842 | 29.559 | 1.00 | 0.00 |
| ATOM | 2104 | C | CYS | 2 | 750 | 16.754 | 72.214 | 30.008 | 1.00 | 0.00 |
| ATOM | 2105 | O | CYS | 2 | 750 | 17.281 | 71.474 | 30.825 | 1.00 | 0.00 |
| ATOM | 2106 | CB | CYS | 2 | 750 | 14.327 | 72.947 | 29.862 | 1.00 | 0.00 |
| ATOM | 2107 | SG | CYS | 2 | 750 | 14.008 | 73.318 | 31.608 | 1.00 | 0.00 |
| ATOM | 2108 | H | CYS | 2 | 750 | 14.736 | 69.789 | 29.409 | 1.00 | 0.00 |
| ATOM | 2109 | N | ASN | 2 | 751 | 17.373 | 73.299 | 29.496 | 1.00 | 0.00 |
| ATOM | 2110 | CA | ASN | 2 | 751 | 18.755 | 73.443 | 29.989 | 1.00 | 0.00 |
| ATOM | 2111 | C | ASN | 2 | 751 | 18.910 | 73.690 | 31.488 | 1.00 | 0.00 |
| ATOM | 2112 | O | ASN | 2 | 751 | 18.057 | 74.318 | 32.118 | 1.00 | 0.00 |
| ATOM | 2113 | CB | ASN | 2 | 751 | 19.631 | 74.354 | 29.103 | 1.00 | 0.00 |
| ATOM | 2114 | CG | ASN | 2 | 751 | 19.558 | 75.866 | 29.316 | 1.00 | 0.00 |
| ATOM | 2115 | OD1 | ASN | 2 | 751 | 20.341 | 76.610 | 28.728 | 1.00 | 0.00 |
| ATOM | 2116 | ND2 | ASN | 2 | 751 | 18.603 | 76.367 | 30.116 | 1.00 | 0.00 |
| ATOM | 2117 | H | ASN | 2 | 751 | 16.944 | 73.882 | 28.804 | 1.00 | 0.00 |
| ATOM | 2118 | 1HD2 | ASN | 2 | 751 | 18.447 | 77.351 | 30.204 | 1.00 | 0.00 |
| ATOM | 2119 | 2HD2 | ASN | 2 | 751 | 18.055 | 75.782 | 30.720 | 1.00 | 0.00 |
| ATOM | 2120 | N | LEU | 2 | 752 | 20.007 | 73.125 | 32.032 | 1.00 | 0.00 |
| ATOM | 2121 | CA | LEU | 2 | 752 | 20.141 | 72.949 | 33.484 | 1.00 | 0.00 |
| ATOM | 2122 | C | LEU | 2 | 752 | 21.527 | 72.452 | 33.886 | 1.00 | 0.00 |
| ATOM | 2123 | O | LEU | 2 | 752 | 21.851 | 71.270 | 33.729 | 1.00 | 0.00 |
| ATOM | 2124 | CB | LEU | 2 | 752 | 19.003 | 72.060 | 34.055 | 1.00 | 0.00 |
| ATOM | 2125 | CG | LEU | 2 | 752 | 18.994 | 70.527 | 33.857 | 1.00 | 0.00 |
| ATOM | 2126 | CD1 | LEU | 2 | 752 | 17.750 | 69.906 | 34.468 | 1.00 | 0.00 |
| ATOM | 2127 | CD2 | LEU | 2 | 752 | 19.153 | 70.020 | 32.428 | 1.00 | 0.00 |
| ATOM | 2128 | H | LEU | 2 | 752 | 20.716 | 72.756 | 31.430 | 1.00 | 0.00 |
| ATOM | 2129 | N | THR | 2 | 753 | 22.342 | 73.422 | 34.335 | 1.00 | 0.00 |
| ATOM | 2130 | CA | THR | 2 | 753 | 23.720 | 73.145 | 34.742 | 1.00 | 0.00 |
| ATOM | 2131 | C | THR | 2 | 753 | 24.437 | 74.405 | 35.197 | 1.00 | 0.00 |
| ATOM | 2132 | O | THR | 2 | 753 | 24.337 | 75.457 | 34.562 | 1.00 | 0.00 |
| ATOM | 2133 | CB | THR | 2 | 753 | 24.496 | 72.422 | 33.616 | 1.00 | 0.00 |
| ATOM | 2134 | OG1 | THR | 2 | 753 | 25.563 | 71.627 | 34.148 | 1.00 | 0.00 |
| ATOM | 2135 | CG2 | THR | 2 | 753 | 24.958 | 73.296 | 32.444 | 1.00 | 0.00 |
| ATOM | 2136 | H | THR | 2 | 753 | 21.937 | 74.302 | 34.570 | 1.00 | 0.00 |
| ATOM | 2137 | HG1 | THR | 2 | 753 | 26.352 | 72.150 | 34.012 | 1.00 | 0.00 |
| ATOM | 2138 | N | GLN | 2 | 754 | 25.168 | 74.265 | 36.306 | 1.00 | 0.00 |
| ATOM | 2139 | CA | GLN | 2 | 754 | 26.176 | 75.272 | 36.621 | 1.00 | 0.00 |
| ATOM | 2140 | C | GLN | 2 | 754 | 27.561 | 74.713 | 36.365 | 1.00 | 0.00 |
| ATOM | 2141 | O | GLN | 2 | 754 | 28.151 | 74.021 | 37.201 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2142 | CB | GLN | 2 | 754 | 26.032 | 75.751 | 38.070 | 1.00 | 0.00 |
| ATOM | 2143 | CG | GLN | 2 | 754 | 26.937 | 76.912 | 38.497 | 1.00 | 0.00 |
| ATOM | 2144 | CD | GLN | 2 | 754 | 26.102 | 78.117 | 38.892 | 1.00 | 0.00 |
| ATOM | 2145 | OE1 | GLN | 2 | 754 | 26.027 | 79.114 | 38.182 | 1.00 | 0.00 |
| ATOM | 2146 | NE2 | GLN | 2 | 754 | 25.489 | 78.023 | 40.071 | 1.00 | 0.00 |
| ATOM | 2147 | H | GLN | 2 | 754 | 25.119 | 73.387 | 36.772 | 1.00 | 0.00 |
| ATOM | 2148 | 1HE2 | GLN | 2 | 754 | 24.959 | 78.793 | 40.428 | 1.00 | 0.00 |
| ATOM | 2149 | 2HE2 | GLN | 2 | 754 | 25.626 | 77.181 | 40.590 | 1.00 | 0.00 |
| ATOM | 2150 | N | ILE | 2 | 755 | 28.052 | 75.038 | 35.162 | 1.00 | 0.00 |
| ATOM | 2151 | CA | ILE | 2 | 755 | 29.424 | 74.754 | 34.729 | 1.00 | 0.00 |
| ATOM | 2152 | C | ILE | 2 | 755 | 29.804 | 73.288 | 34.513 | 1.00 | 0.00 |
| ATOM | 2153 | O | ILE | 2 | 755 | 30.156 | 72.905 | 33.402 | 1.00 | 0.00 |
| ATOM | 2154 | CB | ILE | 2 | 755 | 30.455 | 75.520 | 35.587 | 1.00 | 0.00 |
| ATOM | 2155 | CG1 | ILE | 2 | 755 | 30.103 | 77.013 | 35.575 | 1.00 | 0.00 |
| ATOM | 2156 | CG2 | ILE | 2 | 755 | 31.885 | 75.312 | 35.065 | 1.00 | 0.00 |
| ATOM | 2157 | CD1 | ILE | 2 | 755 | 31.004 | 77.872 | 36.465 | 1.00 | 0.00 |
| ATOM | 2158 | H | ILE | 2 | 755 | 27.460 | 75.630 | 34.619 | 1.00 | 0.00 |
| ATOM | 2159 | N | GLY | 2 | 756 | 29.744 | 72.477 | 35.572 | 1.00 | 0.00 |
| ATOM | 2160 | CA | GLY | 2 | 756 | 30.204 | 71.093 | 35.437 | 1.00 | 0.00 |
| ATOM | 2161 | C | GLY | 2 | 756 | 31.683 | 70.913 | 35.739 | 1.00 | 0.00 |
| ATOM | 2162 | O | GLY | 2 | 756 | 32.291 | 71.728 | 36.439 | 1.00 | 0.00 |
| ATOM | 2163 | H | GLY | 2 | 756 | 29.447 | 72.849 | 36.443 | 1.00 | 0.00 |
| ATOM | 2164 | N | GLY | 2 | 757 | 32.220 | 69.807 | 35.159 | 1.00 | 0.00 |
| ATOM | 2165 | CA | GLY | 2 | 757 | 33.666 | 69.523 | 35.106 | 1.00 | 0.00 |
| ATOM | 2166 | C | GLY | 2 | 757 | 33.988 | 68.113 | 34.584 | 1.00 | 0.00 |
| ATOM | 2167 | O | GLY | 2 | 757 | 33.185 | 67.193 | 34.722 | 1.00 | 0.00 |
| ATOM | 2168 | H | GLY | 2 | 757 | 31.592 | 69.124 | 34.785 | 1.00 | 0.00 |
| ATOM | 2169 | N | LEU | 2 | 758 | 35.181 | 67.942 | 33.978 | 1.00 | 0.00 |
| ATOM | 2170 | CA | LEU | 2 | 758 | 35.500 | 66.643 | 33.339 | 1.00 | 0.00 |
| ATOM | 2171 | C | LEU | 2 | 758 | 35.430 | 65.382 | 34.215 | 1.00 | 0.00 |
| ATOM | 2172 | O | LEU | 2 | 758 | 35.250 | 65.510 | 35.435 | 1.00 | 0.00 |
| ATOM | 2173 | CB | LEU | 2 | 758 | 36.821 | 66.747 | 32.558 | 1.00 | 0.00 |
| ATOM | 2174 | CG | LEU | 2 | 758 | 38.050 | 67.267 | 33.321 | 1.00 | 0.00 |
| ATOM | 2175 | CD1 | LEU | 2 | 758 | 38.634 | 66.265 | 34.321 | 1.00 | 0.00 |
| ATOM | 2176 | CD2 | LEU | 2 | 758 | 39.123 | 67.755 | 32.346 | 1.00 | 0.00 |
| ATOM | 2177 | H | LEU | 2 | 758 | 35.844 | 68.688 | 34.033 | 1.00 | 0.00 |
| ATOM | 2178 | N | ILE | 2 | 759 | 35.552 | 64.196 | 33.538 | 1.00 | 0.00 |
| ATOM | 2179 | CA | ILE | 2 | 759 | 35.527 | 62.876 | 34.205 | 1.00 | 0.00 |
| ATOM | 2180 | C | ILE | 2 | 759 | 35.851 | 61.614 | 33.344 | 1.00 | 0.00 |
| ATOM | 2181 | O | ILE | 2 | 759 | 36.066 | 61.666 | 32.129 | 1.00 | 0.00 |
| ATOM | 2182 | CB | ILE | 2 | 759 | 34.186 | 62.743 | 34.960 | 1.00 | 0.00 |
| ATOM | 2183 | CG1 | ILE | 2 | 759 | 34.303 | 62.167 | 36.377 | 1.00 | 0.00 |
| ATOM | 2184 | CG2 | ILE | 2 | 759 | 33.141 | 62.004 | 34.111 | 1.00 | 0.00 |
| ATOM | 2185 | CD1 | ILE | 2 | 759 | 35.244 | 62.926 | 37.313 | 1.00 | 0.00 |
| ATOM | 2186 | H | ILE | 2 | 759 | 35.566 | 64.242 | 32.538 | 1.00 | 0.00 |
| ATOM | 2187 | N | ASP | 2 | 760 | 35.866 | 60.447 | 34.040 | 1.00 | 0.00 |
| ATOM | 2188 | CA | ASP | 2 | 760 | 35.674 | 59.054 | 33.573 | 1.00 | 0.00 |
| ATOM | 2189 | C | ASP | 2 | 760 | 35.865 | 58.598 | 32.139 | 1.00 | 0.00 |
| ATOM | 2190 | O | ASP | 2 | 760 | 36.900 | 58.054 | 31.758 | 1.00 | 0.00 |
| ATOM | 2191 | CB | ASP | 2 | 760 | 34.320 | 58.464 | 33.983 | 1.00 | 0.00 |
| ATOM | 2192 | CG | ASP | 2 | 760 | 34.146 | 58.398 | 35.468 | 1.00 | 0.00 |
| ATOM | 2193 | OD1 | ASP | 2 | 760 | 33.427 | 59.239 | 35.984 | 1.00 | 0.00 |
| ATOM | 2194 | OD2 | ASP | 2 | 760 | 34.702 | 57.499 | 36.089 | 1.00 | 0.00 |
| ATOM | 2195 | H | ASP | 2 | 760 | 36.005 | 60.544 | 35.024 | 1.00 | 0.00 |
| ATOM | 2196 | N | SER | 2 | 761 | 34.781 | 58.712 | 31.355 | 1.00 | 0.00 |
| ATOM | 2197 | CA | SER | 2 | 761 | 34.870 | 57.991 | 30.091 | 1.00 | 0.00 |
| ATOM | 2198 | C | SER | 2 | 761 | 35.330 | 58.809 | 28.909 | 1.00 | 0.00 |
| ATOM | 2199 | O | SER | 2 | 761 | 36.448 | 58.642 | 28.416 | 1.00 | 0.00 |
| ATOM | 2200 | CB | SER | 2 | 761 | 33.607 | 57.165 | 29.783 | 1.00 | 0.00 |
| ATOM | 2201 | OG | SER | 2 | 761 | 33.504 | 56.001 | 30.635 | 1.00 | 0.00 |
| ATOM | 2202 | H | SER | 2 | 761 | 33.982 | 59.245 | 31.632 | 1.00 | 0.00 |
| ATOM | 2203 | HG | SER | 2 | 761 | 33.635 | 56.340 | 31.520 | 1.00 | 0.00 |
| ATOM | 2204 | N | LYS | 2 | 762 | 34.414 | 59.675 | 28.443 | 1.00 | 0.00 |
| ATOM | 2205 | CA | LYS | 2 | 762 | 34.645 | 60.272 | 27.133 | 1.00 | 0.00 |
| ATOM | 2206 | C | LYS | 2 | 762 | 35.799 | 61.249 | 27.035 | 1.00 | 0.00 |
| ATOM | 2207 | O | LYS | 2 | 762 | 35.691 | 62.448 | 27.314 | 1.00 | 0.00 |
| ATOM | 2208 | CB | LYS | 2 | 762 | 33.347 | 60.851 | 26.550 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2209 | CG | LYS | 2 | 762 | 32.198 | 59.832 | 26.471 | 1.00 | 0.00 |
| ATOM | 2210 | CD | LYS | 2 | 762 | 31.309 | 59.814 | 27.712 | 1.00 | 0.00 |
| ATOM | 2211 | CE | LYS | 2 | 762 | 30.602 | 58.487 | 27.994 | 1.00 | 0.00 |
| ATOM | 2212 | NZ | LYS | 2 | 762 | 29.792 | 58.618 | 29.209 | 1.00 | 0.00 |
| ATOM | 2213 | H | LYS | 2 | 762 | 33.637 | 59.943 | 29.010 | 1.00 | 0.00 |
| ATOM | 2214 | 1HZ | LYS | 2 | 762 | 29.323 | 57.725 | 29.446 | 1.00 | 0.00 |
| ATOM | 2215 | 2HZ | LYS | 2 | 762 | 30.361 | 58.902 | 30.035 | 1.00 | 0.00 |
| ATOM | 2216 | 3HZ | LYS | 2 | 762 | 29.062 | 59.335 | 29.050 | 1.00 | 0.00 |
| ATOM | 2217 | N | GLY | 2 | 763 | 36.894 | 60.668 | 26.554 | 1.00 | 0.00 |
| ATOM | 2218 | CA | GLY | 2 | 763 | 38.052 | 61.440 | 26.160 | 1.00 | 0.00 |
| ATOM | 2219 | C | GLY | 2 | 763 | 38.838 | 60.554 | 25.233 | 1.00 | 0.00 |
| ATOM | 2220 | O | GLY | 2 | 763 | 39.038 | 60.839 | 24.051 | 1.00 | 0.00 |
| ATOM | 2221 | H | GLY | 2 | 763 | 36.875 | 59.667 | 26.526 | 1.00 | 0.00 |
| ATOM | 2222 | N | TYR | 2 | 764 | 39.241 | 59.457 | 25.865 | 1.00 | 0.00 |
| ATOM | 2223 | CA | TYR | 2 | 764 | 39.661 | 58.316 | 25.088 | 1.00 | 0.00 |
| ATOM | 2224 | C | TYR | 2 | 764 | 38.429 | 57.738 | 24.397 | 1.00 | 0.00 |
| ATOM | 2225 | O | TYR | 2 | 764 | 37.342 | 57.636 | 24.972 | 1.00 | 0.00 |
| ATOM | 2226 | CB | TYR | 2 | 764 | 40.345 | 57.331 | 26.054 | 1.00 | 0.00 |
| ATOM | 2227 | CG | TYR | 2 | 764 | 41.509 | 57.930 | 26.854 | 1.00 | 0.00 |
| ATOM | 2228 | CD1 | TYR | 2 | 764 | 42.163 | 59.116 | 26.450 | 1.00 | 0.00 |
| ATOM | 2229 | CD2 | TYR | 2 | 764 | 41.943 | 57.243 | 28.006 | 1.00 | 0.00 |
| ATOM | 2230 | CE1 | TYR | 2 | 764 | 43.290 | 59.579 | 27.151 | 1.00 | 0.00 |
| ATOM | 2231 | CE2 | TYR | 2 | 764 | 43.060 | 57.712 | 28.725 | 1.00 | 0.00 |
| ATOM | 2232 | CZ | TYR | 2 | 764 | 43.746 | 58.855 | 28.267 | 1.00 | 0.00 |
| ATOM | 2233 | OH | TYR | 2 | 764 | 44.911 | 59.259 | 28.903 | 1.00 | 0.00 |
| ATOM | 2234 | H | TYR | 2 | 764 | 38.917 | 59.300 | 26.793 | 1.00 | 0.00 |
| ATOM | 2235 | HH | TYR | 2 | 764 | 44.815 | 59.126 | 29.847 | 1.00 | 0.00 |
| ATOM | 2236 | N | GLY | 2 | 765 | 38.637 | 57.394 | 23.117 | 1.00 | 0.00 |
| ATOM | 2237 | CA | GLY | 2 | 765 | 37.504 | 56.837 | 22.378 | 1.00 | 0.00 |
| ATOM | 2238 | C | GLY | 2 | 765 | 37.849 | 55.723 | 21.415 | 1.00 | 0.00 |
| ATOM | 2239 | O | GLY | 2 | 765 | 37.104 | 54.780 | 21.164 | 1.00 | 0.00 |
| ATOM | 2240 | H | GLY | 2 | 765 | 39.422 | 57.835 | 22.683 | 1.00 | 0.00 |
| ATOM | 2241 | N | VAL | 2 | 766 | 39.041 | 55.863 | 20.824 | 1.00 | 0.00 |
| ATOM | 2242 | CA | VAL | 2 | 766 | 39.434 | 54.760 | 19.957 | 1.00 | 0.00 |
| ATOM | 2243 | C | VAL | 2 | 766 | 40.371 | 53.807 | 20.678 | 1.00 | 0.00 |
| ATOM | 2244 | O | VAL | 2 | 766 | 41.218 | 54.266 | 21.445 | 1.00 | 0.00 |
| ATOM | 2245 | CB | VAL | 2 | 766 | 39.991 | 55.287 | 18.623 | 1.00 | 0.00 |
| ATOM | 2246 | CG1 | VAL | 2 | 766 | 39.949 | 54.221 | 17.529 | 1.00 | 0.00 |
| ATOM | 2247 | CG2 | VAL | 2 | 766 | 39.241 | 56.530 | 18.138 | 1.00 | 0.00 |
| ATOM | 2248 | H | VAL | 2 | 766 | 39.675 | 56.581 | 21.101 | 1.00 | 0.00 |
| ATOM | 2249 | N | GLY | 2 | 767 | 40.156 | 52.495 | 20.416 | 1.00 | 0.00 |
| ATOM | 2250 | CA | GLY | 2 | 767 | 40.852 | 51.410 | 21.130 | 1.00 | 0.00 |
| ATOM | 2251 | C | GLY | 2 | 767 | 41.793 | 50.539 | 20.315 | 1.00 | 0.00 |
| ATOM | 2252 | O | GLY | 2 | 767 | 41.775 | 50.586 | 19.081 | 1.00 | 0.00 |
| ATOM | 2253 | H | GLY | 2 | 767 | 39.442 | 52.282 | 19.748 | 1.00 | 0.00 |
| ATOM | 2254 | N | THR | 2 | 768 | 42.640 | 49.785 | 21.069 | 1.00 | 0.00 |
| ATOM | 2255 | CA | THR | 2 | 768 | 43.720 | 48.849 | 20.664 | 1.00 | 0.00 |
| ATOM | 2256 | C | THR | 2 | 768 | 44.875 | 48.722 | 21.666 | 1.00 | 0.00 |
| ATOM | 2257 | O | THR | 2 | 768 | 45.870 | 49.461 | 21.595 | 1.00 | 0.00 |
| ATOM | 2258 | CB | THR | 2 | 768 | 44.307 | 49.089 | 19.250 | 1.00 | 0.00 |
| ATOM | 2259 | OG1 | THR | 2 | 768 | 45.303 | 48.100 | 18.896 | 1.00 | 0.00 |
| ATOM | 2260 | CG2 | THR | 2 | 768 | 44.863 | 50.501 | 19.059 | 1.00 | 0.00 |
| ATOM | 2261 | H | THR | 2 | 768 | 42.259 | 49.731 | 21.992 | 1.00 | 0.00 |
| ATOM | 2262 | HG1 | THR | 2 | 768 | 45.984 | 48.120 | 19.575 | 1.00 | 0.00 |
| ATOM | 2263 | N | PRO | 2 | 769 | 44.724 | 47.716 | 22.574 | 1.00 | 0.00 |
| ATOM | 2264 | CA | PRO | 2 | 769 | 45.762 | 47.470 | 23.589 | 1.00 | 0.00 |
| ATOM | 2265 | C | PRO | 2 | 769 | 47.148 | 47.372 | 22.983 | 1.00 | 0.00 |
| ATOM | 2266 | O | PRO | 2 | 769 | 47.287 | 46.972 | 21.828 | 1.00 | 0.00 |
| ATOM | 2267 | CB | PRO | 2 | 769 | 45.305 | 46.164 | 24.242 | 1.00 | 0.00 |
| ATOM | 2268 | CG | PRO | 2 | 769 | 43.793 | 46.138 | 24.044 | 1.00 | 0.00 |
| ATOM | 2269 | CD | PRO | 2 | 769 | 43.614 | 46.771 | 22.670 | 1.00 | 0.00 |
| ATOM | 2270 | N | MET | 2 | 770 | 48.161 | 47.804 | 23.769 | 1.00 | 0.00 |
| ATOM | 2271 | CA | MET | 2 | 770 | 49.582 | 47.836 | 23.363 | 1.00 | 0.00 |
| ATOM | 2272 | C | MET | 2 | 770 | 49.928 | 47.469 | 21.914 | 1.00 | 0.00 |
| ATOM | 2273 | O | MET | 2 | 770 | 50.042 | 48.361 | 21.069 | 1.00 | 0.00 |
| ATOM | 2274 | CB | MET | 2 | 770 | 50.448 | 47.099 | 24.390 | 1.00 | 0.00 |
| ATOM | 2275 | CG | MET | 2 | 770 | 50.262 | 47.654 | 25.805 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2276 | SD | MET | 2 | 770 | 51.304 | 46.835 | 27.023 | 1.00 | 0.00 |
| ATOM | 2277 | CE | MET | 2 | 770 | 52.892 | 47.489 | 26.485 | 1.00 | 0.00 |
| ATOM | 2278 | H | MET | 2 | 770 | 47.873 | 48.164 | 24.657 | 1.00 | 0.00 |
| ATOM | 2279 | N | GLY | 2 | 771 | 50.006 | 46.151 | 21.646 | 1.00 | 0.00 |
| ATOM | 2280 | CA | GLY | 2 | 771 | 49.730 | 45.592 | 20.313 | 1.00 | 0.00 |
| ATOM | 2281 | C | GLY | 2 | 771 | 50.529 | 45.997 | 19.077 | 1.00 | 0.00 |
| ATOM | 2282 | O | GLY | 2 | 771 | 51.738 | 45.775 | 18.983 | 1.00 | 0.00 |
| ATOM | 2283 | H | GLY | 2 | 771 | 49.961 | 45.566 | 22.453 | 1.00 | 0.00 |
| ATOM | 2284 | N | SER | 2 | 772 | 49.736 | 46.517 | 18.122 | 1.00 | 0.00 |
| ATOM | 2285 | CA | SER | 2 | 772 | 50.110 | 46.471 | 16.706 | 1.00 | 0.00 |
| ATOM | 2286 | C | SER | 2 | 772 | 50.052 | 47.861 | 16.037 | 1.00 | 0.00 |
| ATOM | 2287 | O | SER | 2 | 772 | 49.698 | 48.841 | 16.692 | 1.00 | 0.00 |
| ATOM | 2288 | CB | SER | 2 | 772 | 49.158 | 45.452 | 16.055 | 1.00 | 0.00 |
| ATOM | 2289 | OG | SER | 2 | 772 | 48.940 | 44.292 | 16.881 | 1.00 | 0.00 |
| ATOM | 2290 | H | SER | 2 | 772 | 48.806 | 46.813 | 18.342 | 1.00 | 0.00 |
| ATOM | 2291 | HG | SER | 2 | 772 | 48.031 | 44.368 | 17.188 | 1.00 | 0.00 |
| ATOM | 2292 | N | PRO | 2 | 773 | 50.425 | 47.983 | 14.720 | 1.00 | 0.00 |
| ATOM | 2293 | CA | PRO | 2 | 773 | 50.177 | 49.261 | 14.018 | 1.00 | 0.00 |
| ATOM | 2294 | C | PRO | 2 | 773 | 48.694 | 49.567 | 13.807 | 1.00 | 0.00 |
| ATOM | 2295 | O | PRO | 2 | 773 | 47.992 | 48.991 | 12.965 | 1.00 | 0.00 |
| ATOM | 2296 | CB | PRO | 2 | 773 | 50.963 | 49.091 | 12.713 | 1.00 | 0.00 |
| ATOM | 2297 | CG | PRO | 2 | 773 | 51.007 | 47.586 | 12.465 | 1.00 | 0.00 |
| ATOM | 2298 | CD | PRO | 2 | 773 | 51.137 | 47.024 | 13.874 | 1.00 | 0.00 |
| ATOM | 2299 | N | TYR | 2 | 774 | 48.242 | 50.469 | 14.681 | 1.00 | 0.00 |
| ATOM | 2300 | CA | TYR | 2 | 774 | 46.850 | 50.529 | 15.107 | 1.00 | 0.00 |
| ATOM | 2301 | C | TYR | 2 | 774 | 46.548 | 51.845 | 15.796 | 1.00 | 0.00 |
| ATOM | 2302 | O | TYR | 2 | 774 | 45.652 | 52.588 | 15.396 | 1.00 | 0.00 |
| ATOM | 2303 | CB | TYR | 2 | 774 | 46.568 | 49.426 | 16.128 | 1.00 | 0.00 |
| ATOM | 2304 | CG | TYR | 2 | 774 | 45.794 | 48.245 | 15.601 | 1.00 | 0.00 |
| ATOM | 2305 | CD1 | TYR | 2 | 774 | 46.507 | 47.152 | 15.085 | 1.00 | 0.00 |
| ATOM | 2306 | CD2 | TYR | 2 | 774 | 44.389 | 48.240 | 15.694 | 1.00 | 0.00 |
| ATOM | 2307 | CE1 | TYR | 2 | 774 | 45.806 | 45.999 | 14.712 | 1.00 | 0.00 |
| ATOM | 2308 | CE2 | TYR | 2 | 774 | 43.679 | 47.094 | 15.308 | 1.00 | 0.00 |
| ATOM | 2309 | CZ | TYR | 2 | 774 | 44.404 | 45.989 | 14.824 | 1.00 | 0.00 |
| ATOM | 2310 | OH | TYR | 2 | 774 | 43.731 | 44.854 | 14.416 | 1.00 | 0.00 |
| ATOM | 2311 | H | TYR | 2 | 774 | 48.939 | 51.149 | 14.946 | 1.00 | 0.00 |
| ATOM | 2312 | HH | TYR | 2 | 774 | 42.894 | 44.804 | 14.885 | 1.00 | 0.00 |
| ATOM | 2313 | N | ARG | 2 | 775 | 47.291 | 52.022 | 16.904 | 1.00 | 0.00 |
| ATOM | 2314 | CA | ARG | 2 | 775 | 47.038 | 53.181 | 17.763 | 1.00 | 0.00 |
| ATOM | 2315 | C | ARG | 2 | 775 | 47.656 | 54.447 | 17.230 | 1.00 | 0.00 |
| ATOM | 2316 | O | ARG | 2 | 775 | 47.194 | 55.563 | 17.424 | 1.00 | 0.00 |
| ATOM | 2317 | CB | ARG | 2 | 775 | 47.499 | 52.901 | 19.188 | 1.00 | 0.00 |
| ATOM | 2318 | CG | ARG | 2 | 775 | 46.957 | 53.868 | 20.249 | 1.00 | 0.00 |
| ATOM | 2319 | CD | ARG | 2 | 775 | 47.185 | 53.387 | 21.687 | 1.00 | 0.00 |
| ATOM | 2320 | NE | ARG | 2 | 775 | 48.606 | 53.258 | 21.995 | 1.00 | 0.00 |
| ATOM | 2321 | CZ | ARG | 2 | 775 | 49.263 | 52.099 | 21.810 | 1.00 | 0.00 |
| ATOM | 2322 | NH1 | ARG | 2 | 775 | 50.585 | 52.115 | 21.743 | 1.00 | 0.00 |
| ATOM | 2323 | NH2 | ARG | 2 | 775 | 48.592 | 50.952 | 21.671 | 1.00 | 0.00 |
| ATOM | 2324 | H | ARG | 2 | 775 | 48.089 | 51.428 | 17.012 | 1.00 | 0.00 |
| ATOM | 2325 | HE | ARG | 2 | 775 | 49.115 | 54.068 | 22.279 | 1.00 | 0.00 |
| ATOM | 2326 | 1HH1 | ARG | 2 | 775 | 51.117 | 51.297 | 21.554 | 1.00 | 0.00 |
| ATOM | 2327 | 2HH1 | ARG | 2 | 775 | 51.072 | 52.976 | 21.862 | 1.00 | 0.00 |
| ATOM | 2328 | 1HH2 | ARG | 2 | 775 | 49.040 | 50.086 | 21.443 | 1.00 | 0.00 |
| ATOM | 2329 | 2HH2 | ARG | 2 | 775 | 47.596 | 50.936 | 21.806 | 1.00 | 0.00 |
| ATOM | 2330 | N | ASP | 2 | 776 | 48.716 | 54.201 | 16.463 | 1.00 | 0.00 |
| ATOM | 2331 | CA | ASP | 2 | 776 | 49.197 | 55.146 | 15.459 | 1.00 | 0.00 |
| ATOM | 2332 | C | ASP | 2 | 776 | 48.121 | 55.524 | 14.461 | 1.00 | 0.00 |
| ATOM | 2333 | O | ASP | 2 | 776 | 47.797 | 56.702 | 14.326 | 1.00 | 0.00 |
| ATOM | 2334 | CB | ASP | 2 | 776 | 50.457 | 54.614 | 14.759 | 1.00 | 0.00 |
| ATOM | 2335 | CG | ASP | 2 | 776 | 50.346 | 53.116 | 14.558 | 1.00 | 0.00 |
| ATOM | 2336 | OD1 | ASP | 2 | 776 | 49.859 | 52.675 | 13.527 | 1.00 | 0.00 |
| ATOM | 2337 | OD2 | ASP | 2 | 776 | 50.708 | 52.382 | 15.469 | 1.00 | 0.00 |
| ATOM | 2338 | H | ASP | 2 | 776 | 49.124 | 53.292 | 16.489 | 1.00 | 0.00 |
| ATOM | 2339 | N | LYS | 2 | 777 | 47.536 | 54.499 | 13.818 | 1.00 | 0.00 |
| ATOM | 2340 | CA | LYS | 2 | 777 | 46.425 | 54.828 | 12.930 | 1.00 | 0.00 |
| ATOM | 2341 | C | LYS | 2 | 777 | 45.361 | 55.709 | 13.575 | 1.00 | 0.00 |
| ATOM | 2342 | O | LYS | 2 | 777 | 44.833 | 56.634 | 12.952 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2343 | CB | LYS | 2 | 777 | 45.859 | 53.559 | 12.272 | 1.00 | 0.00 |
| ATOM | 2344 | CG | LYS | 2 | 777 | 45.016 | 53.785 | 11.006 | 1.00 | 0.00 |
| ATOM | 2345 | CD | LYS | 2 | 777 | 43.567 | 54.203 | 11.263 | 1.00 | 0.00 |
| ATOM | 2346 | CE | LYS | 2 | 777 | 43.166 | 55.534 | 10.624 | 1.00 | 0.00 |
| ATOM | 2347 | NZ | LYS | 2 | 777 | 41.952 | 56.009 | 11.293 | 1.00 | 0.00 |
| ATOM | 2348 | H | LYS | 2 | 777 | 47.931 | 53.587 | 13.906 | 1.00 | 0.00 |
| ATOM | 2349 | 1HZ | LYS | 2 | 777 | 42.104 | 56.119 | 12.313 | 1.00 | 0.00 |
| ATOM | 2350 | 2HZ | LYS | 2 | 777 | 41.667 | 56.933 | 10.937 | 1.00 | 0.00 |
| ATOM | 2351 | 3HZ | LYS | 2 | 777 | 41.169 | 55.352 | 11.110 | 1.00 | 0.00 |
| ATOM | 2352 | N | ILE | 2 | 778 | 45.087 | 55.418 | 14.863 | 1.00 | 0.00 |
| ATOM | 2353 | CA | ILE | 2 | 778 | 44.251 | 56.358 | 15.615 | 1.00 | 0.00 |
| ATOM | 2354 | C | ILE | 2 | 778 | 44.796 | 57.773 | 15.549 | 1.00 | 0.00 |
| ATOM | 2355 | O | ILE | 2 | 778 | 44.225 | 58.656 | 14.917 | 1.00 | 0.00 |
| ATOM | 2356 | CB | ILE | 2 | 778 | 44.093 | 55.964 | 17.090 | 1.00 | 0.00 |
| ATOM | 2357 | CG1 | ILE | 2 | 778 | 43.670 | 54.516 | 17.296 | 1.00 | 0.00 |
| ATOM | 2358 | CG2 | ILE | 2 | 778 | 43.097 | 56.914 | 17.749 | 1.00 | 0.00 |
| ATOM | 2359 | CD1 | ILE | 2 | 778 | 43.552 | 54.135 | 18.774 | 1.00 | 0.00 |
| ATOM | 2360 | H | ILE | 2 | 778 | 45.702 | 54.763 | 15.299 | 1.00 | 0.00 |
| ATOM | 2361 | N | THR | 2 | 779 | 45.961 | 57.953 | 16.189 | 1.00 | 0.00 |
| ATOM | 2362 | CA | THR | 2 | 779 | 46.530 | 59.301 | 16.289 | 1.00 | 0.00 |
| ATOM | 2363 | C | THR | 2 | 779 | 46.520 | 60.133 | 15.013 | 1.00 | 0.00 |
| ATOM | 2364 | O | THR | 2 | 779 | 45.926 | 61.210 | 14.971 | 1.00 | 0.00 |
| ATOM | 2365 | CB | THR | 2 | 779 | 47.916 | 59.233 | 16.930 | 1.00 | 0.00 |
| ATOM | 2366 | OG1 | THR | 2 | 779 | 48.513 | 57.938 | 16.690 | 1.00 | 0.00 |
| ATOM | 2367 | CG2 | THR | 2 | 779 | 47.820 | 59.484 | 18.435 | 1.00 | 0.00 |
| ATOM | 2368 | H | THR | 2 | 779 | 46.427 | 57.212 | 16.673 | 1.00 | 0.00 |
| ATOM | 2369 | HG1 | THR | 2 | 779 | 48.747 | 57.936 | 15.762 | 1.00 | 0.00 |
| ATOM | 2370 | N | ILE | 2 | 780 | 47.116 | 59.538 | 13.944 | 1.00 | 0.00 |
| ATOM | 2371 | CA | ILE | 2 | 780 | 47.086 | 60.192 | 12.629 | 1.00 | 0.00 |
| ATOM | 2372 | C | ILE | 2 | 780 | 45.722 | 60.713 | 12.216 | 1.00 | 0.00 |
| ATOM | 2373 | O | ILE | 2 | 780 | 45.545 | 61.907 | 12.077 | 1.00 | 0.00 |
| ATOM | 2374 | CB | ILE | 2 | 780 | 47.775 | 59.379 | 11.497 | 1.00 | 0.00 |
| ATOM | 2375 | CG1 | ILE | 2 | 780 | 47.603 | 60.058 | 10.126 | 1.00 | 0.00 |
| ATOM | 2376 | CG2 | ILE | 2 | 780 | 47.296 | 57.930 | 11.412 | 1.00 | 0.00 |
| ATOM | 2377 | CD1 | ILE | 2 | 780 | 48.092 | 59.249 | 8.922 | 1.00 | 0.00 |
| ATOM | 2378 | H | ILE | 2 | 780 | 47.582 | 58.657 | 14.057 | 1.00 | 0.00 |
| ATOM | 2379 | N | ALA | 2 | 781 | 44.753 | 59.803 | 12.065 | 1.00 | 0.00 |
| ATOM | 2380 | CA | ALA | 2 | 781 | 43.467 | 60.292 | 11.580 | 1.00 | 0.00 |
| ATOM | 2381 | C | ALA | 2 | 781 | 42.553 | 60.877 | 12.625 | 1.00 | 0.00 |
| ATOM | 2382 | O | ALA | 2 | 781 | 41.401 | 61.217 | 12.343 | 1.00 | 0.00 |
| ATOM | 2383 | CB | ALA | 2 | 781 | 42.689 | 59.167 | 10.935 | 1.00 | 0.00 |
| ATOM | 2384 | H | ALA | 2 | 781 | 44.893 | 58.850 | 12.321 | 1.00 | 0.00 |
| ATOM | 2385 | N | ILE | 2 | 782 | 43.069 | 60.882 | 13.863 | 1.00 | 0.00 |
| ATOM | 2386 | CA | ILE | 2 | 782 | 42.253 | 61.529 | 14.871 | 1.00 | 0.00 |
| ATOM | 2387 | C | ILE | 2 | 782 | 42.492 | 63.026 | 14.885 | 1.00 | 0.00 |
| ATOM | 2388 | O | ILE | 2 | 782 | 41.550 | 63.792 | 15.099 | 1.00 | 0.00 |
| ATOM | 2389 | CB | ILE | 2 | 782 | 42.355 | 60.839 | 16.252 | 1.00 | 0.00 |
| ATOM | 2390 | CG1 | ILE | 2 | 782 | 41.070 | 61.008 | 17.061 | 1.00 | 0.00 |
| ATOM | 2391 | CG2 | ILE | 2 | 782 | 43.554 | 61.297 | 17.090 | 1.00 | 0.00 |
| ATOM | 2392 | CD1 | ILE | 2 | 782 | 39.895 | 60.229 | 16.472 | 1.00 | 0.00 |
| ATOM | 2393 | H | ILE | 2 | 782 | 44.032 | 60.692 | 14.039 | 1.00 | 0.00 |
| ATOM | 2394 | N | LEU | 2 | 783 | 43.765 | 63.376 | 14.563 | 1.00 | 0.00 |
| ATOM | 2395 | CA | LEU | 2 | 783 | 44.114 | 64.755 | 14.229 | 1.00 | 0.00 |
| ATOM | 2396 | C | LEU | 2 | 783 | 43.801 | 65.132 | 12.790 | 1.00 | 0.00 |
| ATOM | 2397 | O | LEU | 2 | 783 | 43.255 | 66.201 | 12.544 | 1.00 | 0.00 |
| ATOM | 2398 | CB | LEU | 2 | 783 | 45.567 | 65.103 | 14.563 | 1.00 | 0.00 |
| ATOM | 2399 | CG | LEU | 2 | 783 | 45.755 | 66.628 | 14.618 | 1.00 | 0.00 |
| ATOM | 2400 | CD1 | LEU | 2 | 783 | 45.756 | 67.163 | 16.049 | 1.00 | 0.00 |
| ATOM | 2401 | CD2 | LEU | 2 | 783 | 46.959 | 67.115 | 13.816 | 1.00 | 0.00 |
| ATOM | 2402 | H | LEU | 2 | 783 | 44.450 | 62.656 | 14.433 | 1.00 | 0.00 |
| ATOM | 2403 | N | GLN | 2 | 784 | 44.050 | 64.193 | 11.861 | 1.00 | 0.00 |
| ATOM | 2404 | CA | GLN | 2 | 784 | 43.603 | 64.359 | 10.458 | 1.00 | 0.00 |
| ATOM | 2405 | C | GLN | 2 | 784 | 42.091 | 64.412 | 10.251 | 1.00 | 0.00 |
| ATOM | 2406 | O | GLN | 2 | 784 | 41.522 | 64.344 | 9.159 | 1.00 | 0.00 |
| ATOM | 2407 | CB | GLN | 2 | 784 | 44.148 | 63.273 | 9.523 | 1.00 | 0.00 |
| ATOM | 2408 | CG | GLN | 2 | 784 | 45.650 | 63.288 | 9.225 | 1.00 | 0.00 |
| ATOM | 2409 | CD | GLN | 2 | 784 | 46.021 | 64.403 | 8.271 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2410 | OE1 | GLN | 2 | 784 | 46.129 | 64.241 | 7.056 | 1.00 | 0.00 |
| ATOM | 2411 | NE2 | GLN | 2 | 784 | 46.298 | 65.557 | 8.876 | 1.00 | 0.00 |
| ATOM | 2412 | H | GLN | 2 | 784 | 44.507 | 63.374 | 12.192 | 1.00 | 0.00 |
| ATOM | 2413 | 1HE2 | GLN | 2 | 784 | 46.522 | 66.376 | 8.347 | 1.00 | 0.00 |
| ATOM | 2414 | 2HE2 | GLN | 2 | 784 | 46.364 | 65.658 | 9.874 | 1.00 | 0.00 |
| ATOM | 2415 | N | LEU | 2 | 785 | 41.376 | 64.516 | 11.377 | 1.00 | 0.00 |
| ATOM | 2416 | CA | LEU | 2 | 785 | 40.000 | 64.943 | 11.237 | 1.00 | 0.00 |
| ATOM | 2417 | C | LEU | 2 | 785 | 39.813 | 66.450 | 11.120 | 1.00 | 0.00 |
| ATOM | 2418 | O | LEU | 2 | 785 | 38.796 | 66.928 | 11.597 | 1.00 | 0.00 |
| ATOM | 2419 | CB | LEU | 2 | 785 | 39.164 | 64.465 | 12.429 | 1.00 | 0.00 |
| ATOM | 2420 | CG | LEU | 2 | 785 | 38.961 | 62.964 | 12.591 | 1.00 | 0.00 |
| ATOM | 2421 | CD1 | LEU | 2 | 785 | 38.399 | 62.649 | 13.974 | 1.00 | 0.00 |
| ATOM | 2422 | CD2 | LEU | 2 | 785 | 38.111 | 62.348 | 11.479 | 1.00 | 0.00 |
| ATOM | 2423 | H | LEU | 2 | 785 | 41.845 | 64.509 | 12.254 | 1.00 | 0.00 |
| ATOM | 2424 | N | GLN | 2 | 786 | 40.756 | 67.213 | 10.552 | 1.00 | 0.00 |
| ATOM | 2425 | CA | GLN | 2 | 786 | 40.552 | 68.656 | 10.758 | 1.00 | 0.00 |
| ATOM | 2426 | C | GLN | 2 | 786 | 40.672 | 69.628 | 9.577 | 1.00 | 0.00 |
| ATOM | 2427 | O | GLN | 2 | 786 | 40.298 | 70.794 | 9.686 | 1.00 | 0.00 |
| ATOM | 2428 | CB | GLN | 2 | 786 | 41.406 | 69.169 | 11.932 | 1.00 | 0.00 |
| ATOM | 2429 | CG | GLN | 2 | 786 | 40.735 | 69.162 | 13.320 | 1.00 | 0.00 |
| ATOM | 2430 | CD | GLN | 2 | 786 | 40.879 | 67.834 | 14.051 | 1.00 | 0.00 |
| ATOM | 2431 | OE1 | GLN | 2 | 786 | 39.943 | 67.063 | 14.234 | 1.00 | 0.00 |
| ATOM | 2432 | NE2 | GLN | 2 | 786 | 42.100 | 67.621 | 14.539 | 1.00 | 0.00 |
| ATOM | 2433 | H | GLN | 2 | 786 | 41.610 | 66.844 | 10.164 | 1.00 | 0.00 |
| ATOM | 2434 | 1HE2 | GLN | 2 | 786 | 42.255 | 66.799 | 15.086 | 1.00 | 0.00 |
| ATOM | 2435 | 2HE2 | GLN | 2 | 786 | 42.914 | 68.175 | 14.341 | 1.00 | 0.00 |
| ATOM | 2436 | N | GLU | 2 | 787 | 41.222 | 69.124 | 8.469 | 1.00 | 0.00 |
| ATOM | 2437 | CA | GLU | 2 | 787 | 41.816 | 69.935 | 7.390 | 1.00 | 0.00 |
| ATOM | 2438 | C | GLU | 2 | 787 | 40.847 | 70.808 | 6.604 | 1.00 | 0.00 |
| ATOM | 2439 | O | GLU | 2 | 787 | 41.167 | 71.854 | 6.038 | 1.00 | 0.00 |
| ATOM | 2440 | CB | GLU | 2 | 787 | 42.584 | 69.038 | 6.398 | 1.00 | 0.00 |
| ATOM | 2441 | CG | GLU | 2 | 787 | 43.691 | 68.126 | 6.963 | 1.00 | 0.00 |
| ATOM | 2442 | CD | GLU | 2 | 787 | 43.097 | 67.124 | 7.932 | 1.00 | 0.00 |
| ATOM | 2443 | OE1 | GLU | 2 | 787 | 42.321 | 66.270 | 7.517 | 1.00 | 0.00 |
| ATOM | 2444 | OE2 | GLU | 2 | 787 | 43.329 | 67.258 | 9.128 | 1.00 | 0.00 |
| ATOM | 2445 | H | GLU | 2 | 787 | 41.340 | 68.134 | 8.448 | 1.00 | 0.00 |
| ATOM | 2446 | N | GLU | 2 | 788 | 39.623 | 70.301 | 6.606 | 1.00 | 0.00 |
| ATOM | 2447 | CA | GLU | 2 | 788 | 38.468 | 71.020 | 6.082 | 1.00 | 0.00 |
| ATOM | 2448 | C | GLU | 2 | 788 | 37.609 | 71.461 | 7.244 | 1.00 | 0.00 |
| ATOM | 2449 | O | GLU | 2 | 788 | 37.061 | 72.563 | 7.324 | 1.00 | 0.00 |
| ATOM | 2450 | CB | GLU | 2 | 788 | 37.627 | 70.130 | 5.158 | 1.00 | 0.00 |
| ATOM | 2451 | CG | GLU | 2 | 788 | 38.260 | 68.794 | 4.736 | 1.00 | 0.00 |
| ATOM | 2452 | CD | GLU | 2 | 788 | 38.125 | 67.690 | 5.782 | 1.00 | 0.00 |
| ATOM | 2453 | OE1 | GLU | 2 | 788 | 38.162 | 67.922 | 6.995 | 1.00 | 0.00 |
| ATOM | 2454 | OE2 | GLU | 2 | 788 | 37.997 | 66.544 | 5.379 | 1.00 | 0.00 |
| ATOM | 2455 | H | GLU | 2 | 788 | 39.519 | 69.402 | 7.027 | 1.00 | 0.00 |
| ATOM | 2456 | N | GLY | 2 | 789 | 37.537 | 70.512 | 8.177 | 1.00 | 0.00 |
| ATOM | 2457 | CA | GLY | 2 | 789 | 36.921 | 70.804 | 9.454 | 1.00 | 0.00 |
| ATOM | 2458 | C | GLY | 2 | 789 | 36.382 | 69.594 | 10.176 | 1.00 | 0.00 |
| ATOM | 2459 | O | GLY | 2 | 789 | 35.798 | 69.768 | 11.244 | 1.00 | 0.00 |
| ATOM | 2460 | H | GLY | 2 | 789 | 38.038 | 69.667 | 7.993 | 1.00 | 0.00 |
| ATOM | 2461 | N | LYS | 2 | 790 | 36.568 | 68.382 | 9.573 | 1.00 | 0.00 |
| ATOM | 2462 | CA | LYS | 2 | 790 | 35.844 | 67.171 | 10.019 | 1.00 | 0.00 |
| ATOM | 2463 | C | LYS | 2 | 790 | 35.294 | 67.174 | 11.433 | 1.00 | 0.00 |
| ATOM | 2464 | O | LYS | 2 | 790 | 34.093 | 67.289 | 11.613 | 1.00 | 0.00 |
| ATOM | 2465 | CB | LYS | 2 | 790 | 36.596 | 65.846 | 9.809 | 1.00 | 0.00 |
| ATOM | 2466 | CG | LYS | 2 | 790 | 37.030 | 65.477 | 8.393 | 1.00 | 0.00 |
| ATOM | 2467 | CD | LYS | 2 | 790 | 38.086 | 64.363 | 8.376 | 1.00 | 0.00 |
| ATOM | 2468 | CE | LYS | 2 | 790 | 39.086 | 64.420 | 7.211 | 1.00 | 0.00 |
| ATOM | 2469 | NZ | LYS | 2 | 790 | 39.807 | 65.706 | 7.212 | 1.00 | 0.00 |
| ATOM | 2470 | H | LYS | 2 | 790 | 37.072 | 68.369 | 8.708 | 1.00 | 0.00 |
| ATOM | 2471 | 1HZ | LYS | 2 | 790 | 40.159 | 65.975 | 6.275 | 1.00 | 0.00 |
| ATOM | 2472 | 2HZ | LYS | 2 | 790 | 39.149 | 66.475 | 7.444 | 1.00 | 0.00 |
| ATOM | 2473 | 3HZ | LYS | 2 | 790 | 40.636 | 65.721 | 7.846 | 1.00 | 0.00 |
| ATOM | 2474 | N | LEU | 2 | 791 | 36.161 | 67.105 | 12.453 | 1.00 | 0.00 |
| ATOM | 2475 | CA | LEU | 2 | 791 | 35.671 | 67.050 | 13.835 | 1.00 | 0.00 |
| ATOM | 2476 | C | LEU | 2 | 791 | 34.755 | 68.197 | 14.242 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2477 | O | LEU | 2 | 791 | 33.705 | 68.013 | 14.847 | 1.00 | 0.00 |
| ATOM | 2478 | CB | LEU | 2 | 791 | 36.845 | 66.929 | 14.805 | 1.00 | 0.00 |
| ATOM | 2479 | CG | LEU | 2 | 791 | 36.466 | 66.445 | 16.207 | 1.00 | 0.00 |
| ATOM | 2480 | CD1 | LEU | 2 | 791 | 35.975 | 64.996 | 16.199 | 1.00 | 0.00 |
| ATOM | 2481 | CD2 | LEU | 2 | 791 | 37.608 | 66.651 | 17.200 | 1.00 | 0.00 |
| ATOM | 2482 | H | LEU | 2 | 791 | 37.138 | 67.221 | 12.280 | 1.00 | 0.00 |
| ATOM | 2483 | N | HIS | 2 | 792 | 35.156 | 69.410 | 13.822 | 1.00 | 0.00 |
| ATOM | 2484 | CA | HIS | 2 | 792 | 34.229 | 70.550 | 13.929 | 1.00 | 0.00 |
| ATOM | 2485 | C | HIS | 2 | 792 | 32.918 | 70.374 | 13.151 | 1.00 | 0.00 |
| ATOM | 2486 | O | HIS | 2 | 792 | 31.808 | 70.464 | 13.673 | 1.00 | 0.00 |
| ATOM | 2487 | CB | HIS | 2 | 792 | 34.970 | 71.848 | 13.556 | 1.00 | 0.00 |
| ATOM | 2488 | CG | HIS | 2 | 792 | 34.070 | 73.068 | 13.553 | 1.00 | 0.00 |
| ATOM | 2489 | ND1 | HIS | 2 | 792 | 33.786 | 73.809 | 14.643 | 1.00 | 0.00 |
| ATOM | 2490 | CD2 | HIS | 2 | 792 | 33.418 | 73.628 | 12.450 | 1.00 | 0.00 |
| ATOM | 2491 | CE1 | HIS | 2 | 792 | 32.963 | 74.827 | 14.238 | 1.00 | 0.00 |
| ATOM | 2492 | NE2 | HIS | 2 | 792 | 32.737 | 74.716 | 12.890 | 1.00 | 0.00 |
| ATOM | 2493 | H | HIS | 2 | 792 | 36.007 | 69.410 | 13.285 | 1.00 | 0.00 |
| ATOM | 2494 | HD1 | HIS | 2 | 792 | 34.108 | 73.636 | 15.552 | 1.00 | 0.00 |
| ATOM | 2495 | N | MET | 2 | 793 | 33.094 | 70.087 | 11.855 | 1.00 | 0.00 |
| ATOM | 2496 | CA | MET | 2 | 793 | 31.963 | 69.844 | 10.955 | 1.00 | 0.00 |
| ATOM | 2497 | C | MET | 2 | 793 | 31.013 | 68.761 | 11.459 | 1.00 | 0.00 |
| ATOM | 2498 | O | MET | 2 | 793 | 29.820 | 68.708 | 11.166 | 1.00 | 0.00 |
| ATOM | 2499 | CB | MET | 2 | 793 | 32.516 | 69.529 | 9.558 | 1.00 | 0.00 |
| ATOM | 2500 | CG | MET | 2 | 793 | 31.463 | 69.339 | 8.464 | 1.00 | 0.00 |
| ATOM | 2501 | SD | MET | 2 | 793 | 32.181 | 68.982 | 6.853 | 1.00 | 0.00 |
| ATOM | 2502 | CE | MET | 2 | 793 | 30.672 | 68.456 | 6.030 | 1.00 | 0.00 |
| ATOM | 2503 | H | MET | 2 | 793 | 34.020 | 69.972 | 11.514 | 1.00 | 0.00 |
| ATOM | 2504 | N | MET | 2 | 794 | 31.590 | 67.902 | 12.309 | 1.00 | 0.00 |
| ATOM | 2505 | CA | MET | 2 | 794 | 30.853 | 66.777 | 12.852 | 1.00 | 0.00 |
| ATOM | 2506 | C | MET | 2 | 794 | 30.384 | 66.941 | 14.278 | 1.00 | 0.00 |
| ATOM | 2507 | O | MET | 2 | 794 | 29.433 | 66.274 | 14.681 | 1.00 | 0.00 |
| ATOM | 2508 | CB | MET | 2 | 794 | 31.661 | 65.491 | 12.691 | 1.00 | 0.00 |
| ATOM | 2509 | CG | MET | 2 | 794 | 31.744 | 65.092 | 11.218 | 1.00 | 0.00 |
| ATOM | 2510 | SD | MET | 2 | 794 | 32.743 | 63.629 | 10.925 | 1.00 | 0.00 |
| ATOM | 2511 | CE | MET | 2 | 794 | 32.266 | 63.392 | 9.209 | 1.00 | 0.00 |
| ATOM | 2512 | H | MET | 2 | 794 | 32.560 | 68.010 | 12.530 | 1.00 | 0.00 |
| ATOM | 2513 | N | LYS | 2 | 795 | 31.061 | 67.834 | 15.018 | 1.00 | 0.00 |
| ATOM | 2514 | CA | LYS | 2 | 795 | 30.605 | 67.999 | 16.393 | 1.00 | 0.00 |
| ATOM | 2515 | C | LYS | 2 | 795 | 29.262 | 68.669 | 16.519 | 1.00 | 0.00 |
| ATOM | 2516 | O | LYS | 2 | 795 | 28.474 | 68.297 | 17.381 | 1.00 | 0.00 |
| ATOM | 2517 | CB | LYS | 2 | 795 | 31.635 | 68.612 | 17.371 | 1.00 | 0.00 |
| ATOM | 2518 | CG | LYS | 2 | 795 | 32.473 | 69.844 | 16.987 | 1.00 | 0.00 |
| ATOM | 2519 | CD | LYS | 2 | 795 | 31.725 | 71.128 | 16.624 | 1.00 | 0.00 |
| ATOM | 2520 | CE | LYS | 2 | 795 | 31.015 | 71.776 | 17.793 | 1.00 | 0.00 |
| ATOM | 2521 | NZ | LYS | 2 | 795 | 30.022 | 72.743 | 17.317 | 1.00 | 0.00 |
| ATOM | 2522 | H | LYS | 2 | 795 | 31.817 | 68.346 | 14.609 | 1.00 | 0.00 |
| ATOM | 2523 | 1HZ | LYS | 2 | 795 | 29.950 | 73.548 | 17.959 | 1.00 | 0.00 |
| ATOM | 2524 | 2HZ | LYS | 2 | 795 | 30.147 | 73.133 | 16.361 | 1.00 | 0.00 |
| ATOM | 2525 | 3HZ | LYS | 2 | 795 | 29.057 | 72.358 | 17.301 | 1.00 | 0.00 |
| ATOM | 2526 | N | GLU | 2 | 796 | 28.997 | 69.654 | 15.636 | 1.00 | 0.00 |
| ATOM | 2527 | CA | GLU | 2 | 796 | 27.815 | 70.507 | 15.868 | 1.00 | 0.00 |
| ATOM | 2528 | C | GLU | 2 | 796 | 26.481 | 69.784 | 16.118 | 1.00 | 0.00 |
| ATOM | 2529 | O | GLU | 2 | 796 | 25.581 | 70.244 | 16.813 | 1.00 | 0.00 |
| ATOM | 2530 | CB | GLU | 2 | 796 | 27.720 | 71.577 | 14.763 | 1.00 | 0.00 |
| ATOM | 2531 | CG | GLU | 2 | 796 | 27.008 | 72.904 | 15.111 | 1.00 | 0.00 |
| ATOM | 2532 | CD | GLU | 2 | 796 | 27.807 | 73.754 | 16.097 | 1.00 | 0.00 |
| ATOM | 2533 | OE1 | GLU | 2 | 796 | 27.506 | 73.744 | 17.283 | 1.00 | 0.00 |
| ATOM | 2534 | OE2 | GLU | 2 | 796 | 28.767 | 74.419 | 15.717 | 1.00 | 0.00 |
| ATOM | 2535 | H | GLU | 2 | 796 | 29.681 | 69.903 | 14.944 | 1.00 | 0.00 |
| ATOM | 2536 | N | LYS | 2 | 797 | 26.395 | 68.578 | 15.533 | 1.00 | 0.00 |
| ATOM | 2537 | CA | LYS | 2 | 797 | 25.202 | 67.761 | 15.781 | 1.00 | 0.00 |
| ATOM | 2538 | C | LYS | 2 | 797 | 24.942 | 67.318 | 17.224 | 1.00 | 0.00 |
| ATOM | 2539 | O | LYS | 2 | 797 | 23.803 | 67.244 | 17.675 | 1.00 | 0.00 |
| ATOM | 2540 | CB | LYS | 2 | 797 | 25.098 | 66.591 | 14.783 | 1.00 | 0.00 |
| ATOM | 2541 | CG | LYS | 2 | 797 | 26.405 | 66.213 | 14.073 | 1.00 | 0.00 |
| ATOM | 2542 | CD | LYS | 2 | 797 | 26.262 | 65.170 | 12.964 | 1.00 | 0.00 |
| ATOM | 2543 | CE | LYS | 2 | 797 | 27.556 | 64.948 | 12.169 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2544 | NZ | LYS | 2 | 797 | 28.587 | 64.271 | 12.964 | 1.00 | 0.00 |
| ATOM | 2545 | H | LYS | 2 | 797 | 27.191 | 68.304 | 14.990 | 1.00 | 0.00 |
| ATOM | 2546 | 1HZ | LYS | 2 | 797 | 28.985 | 64.842 | 13.734 | 1.00 | 0.00 |
| ATOM | 2547 | 2HZ | LYS | 2 | 797 | 28.259 | 63.349 | 13.310 | 1.00 | 0.00 |
| ATOM | 2548 | 3HZ | LYS | 2 | 797 | 29.360 | 63.965 | 12.342 | 1.00 | 0.00 |
| ATOM | 2549 | N | TRP | 2 | 798 | 26.037 | 67.033 | 17.942 | 1.00 | 0.00 |
| ATOM | 2550 | CA | TRP | 2 | 798 | 25.860 | 66.711 | 19.358 | 1.00 | 0.00 |
| ATOM | 2551 | C | TRP | 2 | 798 | 26.268 | 67.818 | 20.314 | 1.00 | 0.00 |
| ATOM | 2552 | O | TRP | 2 | 798 | 25.589 | 68.147 | 21.283 | 1.00 | 0.00 |
| ATOM | 2553 | CB | TRP | 2 | 798 | 26.596 | 65.419 | 19.699 | 1.00 | 0.00 |
| ATOM | 2554 | CG | TRP | 2 | 798 | 25.756 | 64.232 | 19.306 | 1.00 | 0.00 |
| ATOM | 2555 | CD1 | TRP | 2 | 798 | 24.843 | 63.559 | 20.132 | 1.00 | 0.00 |
| ATOM | 2556 | CD2 | TRP | 2 | 798 | 25.706 | 63.546 | 18.037 | 1.00 | 0.00 |
| ATOM | 2557 | NE1 | TRP | 2 | 798 | 24.253 | 62.530 | 19.467 | 1.00 | 0.00 |
| ATOM | 2558 | CE2 | TRP | 2 | 798 | 24.753 | 62.483 | 18.172 | 1.00 | 0.00 |
| ATOM | 2559 | CE3 | TRP | 2 | 798 | 26.380 | 63.731 | 16.812 | 1.00 | 0.00 |
| ATOM | 2560 | CZ2 | TRP | 2 | 798 | 24.489 | 61.629 | 17.080 | 1.00 | 0.00 |
| ATOM | 2561 | CZ3 | TRP | 2 | 798 | 26.109 | 62.870 | 15.727 | 1.00 | 0.00 |
| ATOM | 2562 | CH2 | TRP | 2 | 798 | 25.168 | 61.827 | 15.859 | 1.00 | 0.00 |
| ATOM | 2563 | H | TRP | 2 | 798 | 26.920 | 67.136 | 17.484 | 1.00 | 0.00 |
| ATOM | 2564 | HE1 | TRP | 2 | 798 | 23.580 | 61.904 | 19.807 | 1.00 | 0.00 |
| ATOM | 2565 | N | TRP | 2 | 799 | 27.450 | 68.364 | 20.016 | 1.00 | 0.00 |
| ATOM | 2566 | CA | TRP | 2 | 799 | 27.962 | 69.399 | 20.902 | 1.00 | 0.00 |
| ATOM | 2567 | C | TRP | 2 | 799 | 28.138 | 70.726 | 20.203 | 1.00 | 0.00 |
| ATOM | 2568 | O | TRP | 2 | 799 | 28.333 | 70.847 | 18.990 | 1.00 | 0.00 |
| ATOM | 2569 | CB | TRP | 2 | 799 | 29.227 | 68.920 | 21.629 | 1.00 | 0.00 |
| ATOM | 2570 | CG | TRP | 2 | 799 | 28.887 | 67.605 | 22.294 | 1.00 | 0.00 |
| ATOM | 2571 | CD1 | TRP | 2 | 799 | 27.999 | 67.406 | 23.364 | 1.00 | 0.00 |
| ATOM | 2572 | CD2 | TRP | 2 | 799 | 29.311 | 66.284 | 21.903 | 1.00 | 0.00 |
| ATOM | 2573 | NE1 | TRP | 2 | 799 | 27.844 | 66.084 | 23.638 | 1.00 | 0.00 |
| ATOM | 2574 | CE2 | TRP | 2 | 799 | 28.634 | 65.350 | 22.758 | 1.00 | 0.00 |
| ATOM | 2575 | CE3 | TRP | 2 | 799 | 30.183 | 65.813 | 20.897 | 1.00 | 0.00 |
| ATOM | 2576 | CZ2 | TRP | 2 | 799 | 28.839 | 63.964 | 22.586 | 1.00 | 0.00 |
| ATOM | 2577 | CZ3 | TRP | 2 | 799 | 30.380 | 64.425 | 20.738 | 1.00 | 0.00 |
| ATOM | 2578 | CH2 | TRP | 2 | 799 | 29.711 | 63.506 | 21.575 | 1.00 | 0.00 |
| ATOM | 2579 | H | TRP | 2 | 799 | 28.012 | 68.129 | 19.226 | 1.00 | 0.00 |
| ATOM | 2580 | HE1 | TRP | 2 | 799 | 27.252 | 65.708 | 24.328 | 1.00 | 0.00 |
| ATOM | 2581 | N | ARG | 2 | 800 | 27.983 | 71.758 | 21.041 | 1.00 | 0.00 |
| ATOM | 2582 | CA | ARG | 2 | 800 | 27.927 | 73.077 | 20.418 | 1.00 | 0.00 |
| ATOM | 2583 | C | ARG | 2 | 800 | 29.231 | 73.821 | 20.605 | 1.00 | 0.00 |
| ATOM | 2584 | O | ARG | 2 | 800 | 30.060 | 73.871 | 19.695 | 1.00 | 0.00 |
| ATOM | 2585 | CB | ARG | 2 | 800 | 26.656 | 73.846 | 20.818 | 1.00 | 0.00 |
| ATOM | 2586 | CG | ARG | 2 | 800 | 25.378 | 73.233 | 20.208 | 1.00 | 0.00 |
| ATOM | 2587 | CD | ARG | 2 | 800 | 24.826 | 72.009 | 20.952 | 1.00 | 0.00 |
| ATOM | 2588 | NE | ARG | 2 | 800 | 24.402 | 70.940 | 20.043 | 1.00 | 0.00 |
| ATOM | 2589 | CZ | ARG | 2 | 800 | 23.595 | 69.955 | 20.501 | 1.00 | 0.00 |
| ATOM | 2590 | NH1 | ARG | 2 | 800 | 23.298 | 68.898 | 19.758 | 1.00 | 0.00 |
| ATOM | 2591 | NH2 | ARG | 2 | 800 | 23.089 | 70.023 | 21.724 | 1.00 | 0.00 |
| ATOM | 2592 | H | ARG | 2 | 800 | 28.049 | 71.561 | 22.018 | 1.00 | 0.00 |
| ATOM | 2593 | HE | ARG | 2 | 800 | 24.852 | 70.846 | 19.141 | 1.00 | 0.00 |
| ATOM | 2594 | 1HH1 | ARG | 2 | 800 | 22.721 | 68.174 | 20.164 | 1.00 | 0.00 |
| ATOM | 2595 | 2HH1 | ARG | 2 | 800 | 23.648 | 68.753 | 18.823 | 1.00 | 0.00 |
| ATOM | 2596 | 1HH2 | ARG | 2 | 800 | 22.608 | 69.202 | 22.076 | 1.00 | 0.00 |
| ATOM | 2597 | 2HH2 | ARG | 2 | 800 | 23.208 | 70.820 | 22.316 | 1.00 | 0.00 |
| ATOM | 2598 | N | GLY | 2 | 801 | 29.444 | 74.282 | 21.841 | 1.00 | 0.00 |
| ATOM | 2599 | CA | GLY | 2 | 801 | 30.839 | 74.485 | 22.196 | 1.00 | 0.00 |
| ATOM | 2600 | C | GLY | 2 | 801 | 31.488 | 73.160 | 22.555 | 1.00 | 0.00 |
| ATOM | 2601 | O | GLY | 2 | 801 | 30.798 | 72.191 | 22.886 | 1.00 | 0.00 |
| ATOM | 2602 | H | GLY | 2 | 801 | 28.731 | 74.337 | 22.533 | 1.00 | 0.00 |
| ATOM | 2603 | N | ASN | 2 | 802 | 32.831 | 73.236 | 22.480 | 1.00 | 0.00 |
| ATOM | 2604 | CA | ASN | 2 | 802 | 33.916 | 72.305 | 22.829 | 1.00 | 0.00 |
| ATOM | 2605 | C | ASN | 2 | 802 | 35.095 | 72.723 | 21.979 | 1.00 | 0.00 |
| ATOM | 2606 | O | ASN | 2 | 802 | 34.907 | 73.537 | 21.068 | 1.00 | 0.00 |
| ATOM | 2607 | CB | ASN | 2 | 802 | 33.600 | 70.816 | 22.641 | 1.00 | 0.00 |
| ATOM | 2608 | CG | ASN | 2 | 802 | 33.081 | 70.291 | 23.964 | 1.00 | 0.00 |
| ATOM | 2609 | OD1 | ASN | 2 | 802 | 32.383 | 70.986 | 24.703 | 1.00 | 0.00 |
| ATOM | 2610 | ND2 | ASN | 2 | 802 | 33.432 | 69.035 | 24.255 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2611 | H | ASN | 2 | 802 | 33.169 | 74.086 | 22.080 | 1.00 | 0.00 |
| ATOM | 2612 | 1HD2 | ASN | 2 | 802 | 33.161 | 68.527 | 25.077 | 1.00 | 0.00 |
| ATOM | 2613 | 2HD2 | ASN | 2 | 802 | 34.043 | 68.578 | 23.599 | 1.00 | 0.00 |
| ATOM | 2614 | N | GLY | 2 | 803 | 36.284 | 72.207 | 22.328 | 1.00 | 0.00 |
| ATOM | 2615 | CA | GLY | 2 | 803 | 37.472 | 72.692 | 21.628 | 1.00 | 0.00 |
| ATOM | 2616 | C | GLY | 2 | 803 | 38.747 | 72.358 | 22.378 | 1.00 | 0.00 |
| ATOM | 2617 | O | GLY | 2 | 803 | 38.697 | 71.790 | 23.466 | 1.00 | 0.00 |
| ATOM | 2618 | H | GLY | 2 | 803 | 36.399 | 71.564 | 23.088 | 1.00 | 0.00 |
| ATOM | 2619 | N | CYS | 2 | 804 | 39.877 | 72.742 | 21.739 | 1.00 | 0.00 |
| ATOM | 2620 | CA | CYS | 2 | 804 | 41.249 | 72.312 | 22.084 | 1.00 | 0.00 |
| ATOM | 2621 | C | CYS | 2 | 804 | 41.587 | 70.928 | 21.559 | 1.00 | 0.00 |
| ATOM | 2622 | O | CYS | 2 | 804 | 40.813 | 69.989 | 21.737 | 1.00 | 0.00 |
| ATOM | 2623 | CB | CYS | 2 | 804 | 41.590 | 72.434 | 23.578 | 1.00 | 0.00 |
| ATOM | 2624 | SG | CYS | 2 | 804 | 41.297 | 74.130 | 24.158 | 1.00 | 0.00 |
| ATOM | 2625 | H | CYS | 2 | 804 | 39.725 | 73.297 | 20.925 | 1.00 | 0.00 |
| ATOM | 2626 | N | PRO | 2 | 805 | 42.720 | 70.872 | 20.809 | 1.00 | 0.00 |
| ATOM | 2627 | CA | PRO | 2 | 805 | 43.220 | 69.590 | 20.300 | 1.00 | 0.00 |
| ATOM | 2628 | C | PRO | 2 | 805 | 44.015 | 68.881 | 21.380 | 1.00 | 0.00 |
| ATOM | 2629 | O | PRO | 2 | 805 | 44.130 | 69.386 | 22.495 | 1.00 | 0.00 |
| ATOM | 2630 | CB | PRO | 2 | 805 | 44.083 | 70.042 | 19.120 | 1.00 | 0.00 |
| ATOM | 2631 | CG | PRO | 2 | 805 | 44.691 | 71.364 | 19.586 | 1.00 | 0.00 |
| ATOM | 2632 | CD | PRO | 2 | 805 | 43.556 | 71.994 | 20.387 | 1.00 | 0.00 |
| ATOM | 2633 | N | GLU | 2 | 806 | 44.529 | 67.702 | 21.000 | 1.00 | 0.00 |
| ATOM | 2634 | CA | GLU | 2 | 806 | 45.201 | 66.847 | 21.970 | 1.00 | 0.00 |
| ATOM | 2635 | C | GLU | 2 | 806 | 46.364 | 66.104 | 21.331 | 1.00 | 0.00 |
| ATOM | 2636 | O | GLU | 2 | 806 | 46.215 | 65.049 | 20.721 | 1.00 | 0.00 |
| ATOM | 2637 | CB | GLU | 2 | 806 | 44.174 | 65.894 | 22.594 | 1.00 | 0.00 |
| ATOM | 2638 | CG | GLU | 2 | 806 | 43.462 | 66.433 | 23.845 | 1.00 | 0.00 |
| ATOM | 2639 | CD | GLU | 2 | 806 | 44.328 | 66.249 | 25.080 | 1.00 | 0.00 |
| ATOM | 2640 | OE1 | GLU | 2 | 806 | 45.423 | 66.805 | 25.141 | 1.00 | 0.00 |
| ATOM | 2641 | OE2 | GLU | 2 | 806 | 43.930 | 65.512 | 25.984 | 1.00 | 0.00 |
| ATOM | 2642 | H | GLU | 2 | 806 | 44.314 | 67.338 | 20.096 | 1.00 | 0.00 |
| ATOM | 2643 | N | GLU | 2 | 807 | 47.540 | 66.746 | 21.485 | 1.00 | 0.00 |
| ATOM | 2644 | CA | GLU | 2 | 807 | 48.866 | 66.269 | 21.050 | 1.00 | 0.00 |
| ATOM | 2645 | C | GLU | 2 | 807 | 49.363 | 66.461 | 19.602 | 1.00 | 0.00 |
| ATOM | 2646 | O | GLU | 2 | 807 | 49.761 | 67.555 | 19.193 | 1.00 | 0.00 |
| ATOM | 2647 | CB | GLU | 2 | 807 | 49.172 | 64.858 | 21.594 | 1.00 | 0.00 |
| ATOM | 2648 | CG | GLU | 2 | 807 | 50.159 | 64.857 | 22.764 | 1.00 | 0.00 |
| ATOM | 2649 | CD | GLU | 2 | 807 | 49.491 | 64.286 | 24.000 | 1.00 | 0.00 |
| ATOM | 2650 | OE1 | GLU | 2 | 807 | 49.025 | 65.056 | 24.830 | 1.00 | 0.00 |
| ATOM | 2651 | OE2 | GLU | 2 | 807 | 49.429 | 63.068 | 24.144 | 1.00 | 0.00 |
| ATOM | 2652 | H | GLU | 2 | 807 | 47.501 | 67.616 | 21.977 | 1.00 | 0.00 |
| ATOM | 2653 | N | GLU | 2 | 808 | 49.432 | 65.317 | 18.893 | 1.00 | 0.00 |
| ATOM | 2654 | CA | GLU | 2 | 808 | 50.376 | 65.174 | 17.775 | 1.00 | 0.00 |
| ATOM | 2655 | C | GLU | 2 | 808 | 50.057 | 65.973 | 16.513 | 1.00 | 0.00 |
| ATOM | 2656 | O | GLU | 2 | 808 | 48.921 | 66.028 | 16.052 | 1.00 | 0.00 |
| ATOM | 2657 | CB | GLU | 2 | 808 | 50.575 | 63.670 | 17.509 | 1.00 | 0.00 |
| ATOM | 2658 | CG | GLU | 2 | 808 | 51.563 | 63.222 | 16.415 | 1.00 | 0.00 |
| ATOM | 2659 | CD | GLU | 2 | 808 | 53.002 | 63.633 | 16.696 | 1.00 | 0.00 |
| ATOM | 2660 | OE1 | GLU | 2 | 808 | 53.858 | 62.780 | 16.924 | 1.00 | 0.00 |
| ATOM | 2661 | OE2 | GLU | 2 | 808 | 53.327 | 64.812 | 16.606 | 1.00 | 0.00 |
| ATOM | 2662 | H | GLU | 2 | 808 | 48.805 | 64.563 | 19.089 | 1.00 | 0.00 |
| ATOM | 2663 | N | SER | 2 | 809 | 51.137 | 66.589 | 15.996 | 1.00 | 0.00 |
| ATOM | 2664 | CA | SER | 2 | 809 | 51.000 | 67.433 | 14.806 | 1.00 | 0.00 |
| ATOM | 2665 | C | SER | 2 | 809 | 52.048 | 67.187 | 13.719 | 1.00 | 0.00 |
| ATOM | 2666 | O | SER | 2 | 809 | 52.513 | 68.089 | 13.015 | 1.00 | 0.00 |
| ATOM | 2667 | CB | SER | 2 | 809 | 50.964 | 68.908 | 15.221 | 1.00 | 0.00 |
| ATOM | 2668 | OG | SER | 2 | 809 | 51.443 | 69.081 | 16.574 | 1.00 | 0.00 |
| ATOM | 2669 | H | SER | 2 | 809 | 52.031 | 66.451 | 16.423 | 1.00 | 0.00 |
| ATOM | 2670 | HG | SER | 2 | 809 | 50.845 | 68.527 | 17.078 | 1.00 | 0.00 |
| ATOM | 2671 | N | LYS | 2 | 810 | 52.446 | 65.901 | 13.655 | 1.00 | 0.00 |
| ATOM | 2672 | CA | LYS | 2 | 810 | 53.137 | 65.311 | 12.504 | 1.00 | 0.00 |
| ATOM | 2673 | C | LYS | 2 | 810 | 52.902 | 63.815 | 12.547 | 1.00 | 0.00 |
| ATOM | 2674 | O | LYS | 2 | 810 | 53.593 | 63.096 | 13.274 | 1.00 | 0.00 |
| ATOM | 2675 | CB | LYS | 2 | 810 | 54.664 | 65.522 | 12.411 | 1.00 | 0.00 |
| ATOM | 2676 | CG | LYS | 2 | 810 | 55.426 | 66.533 | 13.281 | 1.00 | 0.00 |
| ATOM | 2677 | CD | LYS | 2 | 810 | 55.615 | 66.195 | 14.769 | 1.00 | 0.00 |

```
ATOM   2678  CE  LYS 2 810      56.253  64.835  15.095  1.00  0.00
ATOM   2679  NZ  LYS 2 810      55.246  63.776  15.024  1.00  0.00
ATOM   2680  H   LYS 2 810      52.001  65.286  14.307  1.00  0.00
ATOM   2681 1HZ  LYS 2 810      55.335  63.064  15.778  1.00  0.00
ATOM   2682 2HZ  LYS 2 810      54.316  64.192  15.245  1.00  0.00
ATOM   2683 3HZ  LYS 2 810      55.136  63.312  14.100  1.00  0.00
ATOM   2684  N   GLU 2 811      51.881  63.421  11.796  1.00  0.00
ATOM   2685  CA  GLU 2 811      51.096  62.266  12.182  1.00  0.00
ATOM   2686  C   GLU 2 811      51.002  61.260  11.051  1.00  0.00
ATOM   2687  O   GLU 2 811      50.643  61.619   9.936  1.00  0.00
ATOM   2688  CB  GLU 2 811      49.722  62.767  12.690  1.00  0.00
ATOM   2689  CG  GLU 2 811      48.708  63.403  11.701  1.00  0.00
ATOM   2690  CD  GLU 2 811      48.932  64.868  11.325  1.00  0.00
ATOM   2691  OE1 GLU 2 811      47.945  65.580  11.139  1.00  0.00
ATOM   2692  OE2 GLU 2 811      50.072  65.309  11.196  1.00  0.00
ATOM   2693  H   GLU 2 811      51.555  64.015  11.060  1.00  0.00
ATOM   2694  N   ALA 2 812      51.365  60.012  11.388  1.00  0.00
ATOM   2695  CA  ALA 2 812      51.371  58.887  10.449  1.00  0.00
ATOM   2696  C   ALA 2 812      51.803  57.606  11.160  1.00  0.00
ATOM   2697  O   ALA 2 812      52.802  57.659  11.880  1.00  0.00
ATOM   2698  CB  ALA 2 812      52.338  59.111   9.277  1.00  0.00
ATOM   2699  OXT ALA 2 812      51.160  56.561  11.004  1.00  0.00
ATOM   2700  H   ALA 2 812      51.621  59.777  12.323  1.00  0.00
END
```

**TABLE 5**

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| REMARK | 1 | NMDA | Receptor | Model | (NR2) | of | the | NR2-B | Glutamate | Binding Site |
| ATOM | 1 | N | LYS S | 1 | 18.429 | 77.937 | 39.479 | 1.00 | 0.00 | |
| ATOM | 2 | CA | LYS S | 1 | 17.556 | 78.094 | 40.646 | 1.00 | 0.00 | |
| ATOM | 3 | C | LYS S | 1 | 18.237 | 78.854 | 41.768 | 1.00 | 0.00 | |
| ATOM | 4 | O | LYS S | 1 | 17.801 | 79.919 | 42.195 | 1.00 | 0.00 | |
| ATOM | 5 | CB | LYS S | 1 | 17.092 | 76.744 | 41.223 | 1.00 | 0.00 | |
| ATOM | 6 | CG | LYS S | 1 | 15.896 | 76.069 | 40.553 | 1.00 | 0.00 | |
| ATOM | 7 | CD | LYS S | 1 | 15.533 | 74.731 | 41.210 | 1.00 | 0.00 | |
| ATOM | 8 | CE | LYS S | 1 | 14.443 | 73.947 | 40.467 | 1.00 | 0.00 | |
| ATOM | 9 | NZ | LYS S | 1 | 15.017 | 73.031 | 39.467 | 1.00 | 0.00 | |
| ATOM | 10 | 1H | LYS S | 1 | 18.907 | 78.837 | 39.244 | 1.00 | 0.00 | |
| ATOM | 11 | 2H | LYS S | 1 | 19.198 | 77.276 | 39.679 | 1.00 | 0.00 | |
| ATOM | 12 | 3H | LYS S | 1 | 17.921 | 77.602 | 38.635 | 1.00 | 0.00 | |
| ATOM | 13 | 1HZ | LYS S | 1 | 15.718 | 73.497 | 38.853 | 1.00 | 0.00 | |
| ATOM | 14 | 2HZ | LYS S | 1 | 15.434 | 72.214 | 39.954 | 1.00 | 0.00 | |
| ATOM | 15 | 3HZ | LYS S | 1 | 14.285 | 72.655 | 38.831 | 1.00 | 0.00 | |
| ATOM | 16 | N | LYS S | 2 | 19.268 | 78.190 | 42.310 | 1.00 | 0.00 | |
| ATOM | 17 | CA | LYS S | 2 | 19.708 | 78.705 | 43.602 | 1.00 | 0.00 | |
| ATOM | 18 | C | LYS S | 2 | 21.208 | 78.790 | 43.749 | 1.00 | 0.00 | |
| ATOM | 19 | O | LYS S | 2 | 21.733 | 79.700 | 44.404 | 1.00 | 0.00 | |
| ATOM | 20 | CB | LYS S | 2 | 19.039 | 77.894 | 44.733 | 1.00 | 0.00 | |
| ATOM | 21 | CG | LYS S | 2 | 19.268 | 78.411 | 46.162 | 1.00 | 0.00 | |
| ATOM | 22 | CD | LYS S | 2 | 20.533 | 77.847 | 46.819 | 1.00 | 0.00 | |
| ATOM | 23 | CE | LYS S | 2 | 21.235 | 78.842 | 47.748 | 1.00 | 0.00 | |
| ATOM | 24 | NZ | LYS S | 2 | 21.652 | 80.026 | 46.982 | 1.00 | 0.00 | |
| ATOM | 25 | H | LYS S | 2 | 19.635 | 77.361 | 41.892 | 1.00 | 0.00 | |
| ATOM | 26 | 1HZ | LYS S | 2 | 22.358 | 80.561 | 47.519 | 1.00 | 0.00 | |
| ATOM | 27 | 2HZ | LYS S | 2 | 22.062 | 79.762 | 46.061 | 1.00 | 0.00 | |
| ATOM | 28 | 3HZ | LYS S | 2 | 20.828 | 80.624 | 46.781 | 1.00 | 0.00 | |
| ATOM | 29 | N | PHE S | 3 | 21.844 | 77.757 | 43.174 | 1.00 | 0.00 | |
| ATOM | 30 | CA | PHE S | 3 | 23.290 | 77.613 | 43.222 | 1.00 | 0.00 | |
| ATOM | 31 | C | PHE S | 3 | 23.689 | 76.518 | 42.263 | 1.00 | 0.00 | |
| ATOM | 32 | O | PHE S | 3 | 23.019 | 75.490 | 42.141 | 1.00 | 0.00 | |
| ATOM | 33 | CB | PHE S | 3 | 23.802 | 77.317 | 44.641 | 1.00 | 0.00 | |
| ATOM | 34 | CG | PHE S | 3 | 25.264 | 77.690 | 44.767 | 1.00 | 0.00 | |
| ATOM | 35 | CD1 | PHE S | 3 | 26.192 | 76.709 | 45.175 | 1.00 | 0.00 | |
| ATOM | 36 | CD2 | PHE S | 3 | 25.680 | 79.010 | 44.476 | 1.00 | 0.00 | |
| ATOM | 37 | CE1 | PHE S | 3 | 27.556 | 77.044 | 45.278 | 1.00 | 0.00 | |
| ATOM | 38 | CE2 | PHE S | 3 | 27.043 | 79.346 | 44.578 | 1.00 | 0.00 | |
| ATOM | 39 | CZ | PHE S | 3 | 27.969 | 78.357 | 44.971 | 1.00 | 0.00 | |
| ATOM | 40 | H | PHE S | 3 | 21.339 | 77.087 | 42.633 | 1.00 | 0.00 | |
| ATOM | 41 | N | GLN S | 4 | 24.782 | 76.811 | 41.550 | 1.00 | 0.00 | |
| ATOM | 42 | CA | GLN S | 4 | 25.325 | 75.781 | 40.670 | 1.00 | 0.00 | |
| ATOM | 43 | C | GLN S | 4 | 25.863 | 74.681 | 41.564 | 1.00 | 0.00 | |
| ATOM | 44 | O | GLN S | 4 | 26.261 | 74.976 | 42.688 | 1.00 | 0.00 | |
| ATOM | 45 | CB | GLN S | 4 | 26.406 | 76.446 | 39.808 | 1.00 | 0.00 | |
| ATOM | 46 | CG | GLN S | 4 | 27.150 | 75.558 | 38.811 | 1.00 | 0.00 | |
| ATOM | 47 | CD | GLN S | 4 | 28.625 | 75.580 | 39.156 | 1.00 | 0.00 | |
| ATOM | 48 | OE1 | GLN S | 4 | 29.357 | 76.551 | 38.957 | 1.00 | 0.00 | |
| ATOM | 49 | NE2 | GLN S | 4 | 29.061 | 74.465 | 39.739 | 1.00 | 0.00 | |
| ATOM | 50 | H | GLN S | 4 | 25.335 | 77.617 | 41.767 | 1.00 | 0.00 | |
| ATOM | 51 | 1HE2 | GLN S | 4 | 30.013 | 74.361 | 40.014 | 1.00 | 0.00 | |
| ATOM | 52 | 2HE2 | GLN S | 4 | 28.476 | 73.669 | 39.919 | 1.00 | 0.00 | |
| ATOM | 53 | N | ARG S | 5 | 25.847 | 73.428 | 41.079 | 1.00 | 0.00 | |
| ATOM | 54 | CA | ARG S | 5 | 26.355 | 72.361 | 41.948 | 1.00 | 0.00 | |
| ATOM | 55 | C | ARG S | 5 | 27.637 | 72.714 | 42.698 | 1.00 | 0.00 | |
| ATOM | 56 | O | ARG S | 5 | 28.700 | 72.991 | 42.148 | 1.00 | 0.00 | |
| ATOM | 57 | CB | ARG S | 5 | 26.476 | 71.056 | 41.165 | 1.00 | 0.00 | |
| ATOM | 58 | CG | ARG S | 5 | 26.858 | 69.787 | 41.940 | 1.00 | 0.00 | |
| ATOM | 59 | CD | ARG S | 5 | 27.068 | 68.655 | 40.933 | 1.00 | 0.00 | |
| ATOM | 60 | NE | ARG S | 5 | 27.356 | 67.354 | 41.533 | 1.00 | 0.00 | |
| ATOM | 61 | CZ | ARG S | 5 | 27.404 | 66.260 | 40.741 | 1.00 | 0.00 | |
| ATOM | 62 | NH1 | ARG S | 5 | 27.717 | 65.081 | 41.265 | 1.00 | 0.00 | |
| ATOM | 63 | NH2 | ARG S | 5 | 27.167 | 66.351 | 39.437 | 1.00 | 0.00 | |
| ATOM | 64 | H | ARG S | 5 | 25.340 | 73.235 | 40.239 | 1.00 | 0.00 | |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 65 | HE | ARG | S | 5 | 27.737 | 67.231 | 42.450 | 1.00 | 0.00 |
| ATOM | 66 | 1HH1 | ARG | S | 5 | 27.899 | 64.953 | 42.238 | 1.00 | 0.00 |
| ATOM | 67 | 2HH1 | ARG | S | 5 | 27.782 | 64.277 | 40.669 | 1.00 | 0.00 |
| ATOM | 68 | 1HH2 | ARG | S | 5 | 27.284 | 65.561 | 38.816 | 1.00 | 0.00 |
| ATOM | 69 | 2HH2 | ARG | S | 5 | 26.877 | 67.207 | 39.002 | 1.00 | 0.00 |
| ATOM | 70 | N | PRO | S | 6 | 27.446 | 72.765 | 44.032 | 1.00 | 0.00 |
| ATOM | 71 | CA | PRO | S | 6 | 28.582 | 73.136 | 44.864 | 1.00 | 0.00 |
| ATOM | 72 | C | PRO | S | 6 | 29.592 | 72.006 | 44.939 | 1.00 | 0.00 |
| ATOM | 73 | O | PRO | S | 6 | 29.296 | 70.894 | 45.374 | 1.00 | 0.00 |
| ATOM | 74 | CB | PRO | S | 6 | 27.872 | 73.516 | 46.165 | 1.00 | 0.00 |
| ATOM | 75 | CG | PRO | S | 6 | 26.562 | 72.732 | 46.216 | 1.00 | 0.00 |
| ATOM | 76 | CD | PRO | S | 6 | 26.190 | 72.568 | 44.755 | 1.00 | 0.00 |
| ATOM | 77 | N | ASN | S | 7 | 30.786 | 72.308 | 44.437 | 1.00 | 0.00 |
| ATOM | 78 | CA | ASN | S | 7 | 31.865 | 71.324 | 44.516 | 1.00 | 0.00 |
| ATOM | 79 | C | ASN | S | 7 | 33.128 | 71.849 | 45.172 | 1.00 | 0.00 |
| ATOM | 80 | O | ASN | S | 7 | 34.066 | 71.140 | 45.524 | 1.00 | 0.00 |
| ATOM | 81 | CB | ASN | S | 7 | 32.148 | 70.700 | 43.156 | 1.00 | 0.00 |
| ATOM | 82 | CG | ASN | S | 7 | 32.258 | 69.196 | 43.299 | 1.00 | 0.00 |
| ATOM | 83 | OD1 | ASN | S | 7 | 31.726 | 68.446 | 42.488 | 1.00 | 0.00 |
| ATOM | 84 | ND2 | ASN | S | 7 | 32.928 | 68.756 | 44.367 | 1.00 | 0.00 |
| ATOM | 85 | H | ASN | S | 7 | 30.880 | 73.224 | 44.051 | 1.00 | 0.00 |
| ATOM | 86 | 1HD2 | ASN | S | 7 | 33.012 | 67.775 | 44.523 | 1.00 | 0.00 |
| ATOM | 87 | 2HD2 | ASN | S | 7 | 33.402 | 69.360 | 45.011 | 1.00 | 0.00 |
| ATOM | 88 | N | ASP | S | 8 | 33.037 | 73.166 | 45.411 | 1.00 | 0.00 |
| ATOM | 89 | CA | ASP | S | 8 | 33.658 | 73.842 | 46.549 | 1.00 | 0.00 |
| ATOM | 90 | C | ASP | S | 8 | 33.736 | 72.968 | 47.787 | 1.00 | 0.00 |
| ATOM | 91 | O | ASP | S | 8 | 32.756 | 72.634 | 48.459 | 1.00 | 0.00 |
| ATOM | 92 | CB | ASP | S | 8 | 32.910 | 75.157 | 46.834 | 1.00 | 0.00 |
| ATOM | 93 | CG | ASP | S | 8 | 31.406 | 74.970 | 46.682 | 1.00 | 0.00 |
| ATOM | 94 | OD1 | ASP | S | 8 | 30.898 | 75.125 | 45.578 | 1.00 | 0.00 |
| ATOM | 95 | OD2 | ASP | S | 8 | 30.735 | 74.644 | 47.647 | 1.00 | 0.00 |
| ATOM | 96 | H | ASP | S | 8 | 32.360 | 73.699 | 44.914 | 1.00 | 0.00 |
| ATOM | 97 | N | PHE | S | 9 | 34.998 | 72.558 | 47.982 | 1.00 | 0.00 |
| ATOM | 98 | CA | PHE | S | 9 | 35.376 | 71.612 | 49.033 | 1.00 | 0.00 |
| ATOM | 99 | C | PHE | S | 9 | 34.608 | 70.300 | 48.977 | 1.00 | 0.00 |
| ATOM | 100 | O | PHE | S | 9 | 33.853 | 70.034 | 48.037 | 1.00 | 0.00 |
| ATOM | 101 | CB | PHE | S | 9 | 35.297 | 72.273 | 50.422 | 1.00 | 0.00 |
| ATOM | 102 | CG | PHE | S | 9 | 36.133 | 73.532 | 50.468 | 1.00 | 0.00 |
| ATOM | 103 | CD1 | PHE | S | 9 | 35.489 | 74.788 | 50.436 | 1.00 | 0.00 |
| ATOM | 104 | CD2 | PHE | S | 9 | 37.540 | 73.434 | 50.542 | 1.00 | 0.00 |
| ATOM | 105 | CE1 | PHE | S | 9 | 36.262 | 75.964 | 50.470 | 1.00 | 0.00 |
| ATOM | 106 | CE2 | PHE | S | 9 | 38.315 | 74.609 | 50.577 | 1.00 | 0.00 |
| ATOM | 107 | CZ | PHE | S | 9 | 37.668 | 75.863 | 50.539 | 1.00 | 0.00 |
| ATOM | 108 | H | PHE | S | 9 | 35.700 | 72.928 | 47.383 | 1.00 | 0.00 |
| ATOM | 109 | N | SER | S | 10 | 34.791 | 69.508 | 50.051 | 1.00 | 0.00 |
| ATOM | 110 | CA | SER | S | 10 | 34.075 | 68.232 | 50.016 | 1.00 | 0.00 |
| ATOM | 111 | C | SER | S | 10 | 33.073 | 67.918 | 51.137 | 1.00 | 0.00 |
| ATOM | 112 | O | SER | S | 10 | 33.097 | 66.831 | 51.709 | 1.00 | 0.00 |
| ATOM | 113 | CB | SER | S | 10 | 35.117 | 67.115 | 49.878 | 1.00 | 0.00 |
| ATOM | 114 | OG | SER | S | 10 | 36.297 | 67.640 | 49.236 | 1.00 | 0.00 |
| ATOM | 115 | H | SER | S | 10 | 35.497 | 69.685 | 50.731 | 1.00 | 0.00 |
| ATOM | 116 | HG | SER | S | 10 | 36.772 | 66.869 | 48.930 | 1.00 | 0.00 |
| ATOM | 117 | N | PRO | S | 11 | 32.185 | 68.892 | 51.506 | 1.00 | 0.00 |
| ATOM | 118 | CA | PRO | S | 11 | 31.269 | 68.567 | 52.601 | 1.00 | 0.00 |
| ATOM | 119 | C | PRO | S | 11 | 30.090 | 67.706 | 52.158 | 1.00 | 0.00 |
| ATOM | 120 | O | PRO | S | 11 | 29.635 | 67.739 | 51.009 | 1.00 | 0.00 |
| ATOM | 121 | CB | PRO | S | 11 | 30.879 | 69.961 | 53.109 | 1.00 | 0.00 |
| ATOM | 122 | CG | PRO | S | 11 | 30.876 | 70.846 | 51.870 | 1.00 | 0.00 |
| ATOM | 123 | CD | PRO | S | 11 | 31.986 | 70.254 | 51.012 | 1.00 | 0.00 |
| ATOM | 124 | N | PRO | S | 12 | 29.625 | 66.903 | 53.139 | 1.00 | 0.00 |
| ATOM | 125 | CA | PRO | S | 12 | 28.359 | 66.202 | 52.960 | 1.00 | 0.00 |
| ATOM | 126 | C | PRO | S | 12 | 27.186 | 67.166 | 52.921 | 1.00 | 0.00 |
| ATOM | 127 | O | PRO | S | 12 | 27.257 | 68.314 | 53.371 | 1.00 | 0.00 |
| ATOM | 128 | CB | PRO | S | 12 | 28.329 | 65.265 | 54.171 | 1.00 | 0.00 |
| ATOM | 129 | CG | PRO | S | 12 | 29.135 | 65.980 | 55.252 | 1.00 | 0.00 |
| ATOM | 130 | CD | PRO | S | 12 | 30.235 | 66.653 | 54.442 | 1.00 | 0.00 |
| ATOM | 131 | N | PHE | S | 13 | 26.115 | 66.568 | 52.359 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 132 | CA | PHE | S | 13 | 24.839 | 67.215 | 52.030 | 1.00 | 0.00 |
| ATOM | 133 | C | PHE | S | 13 | 24.831 | 67.806 | 50.629 | 1.00 | 0.00 |
| ATOM | 134 | O | PHE | S | 13 | 23.816 | 68.261 | 50.100 | 1.00 | 0.00 |
| ATOM | 135 | CB | PHE | S | 13 | 24.356 | 68.228 | 53.092 | 1.00 | 0.00 |
| ATOM | 136 | CG | PHE | S | 13 | 22.849 | 68.324 | 53.172 | 1.00 | 0.00 |
| ATOM | 137 | CD1 | PHE | S | 13 | 22.161 | 69.278 | 52.389 | 1.00 | 0.00 |
| ATOM | 138 | CD2 | PHE | S | 13 | 22.154 | 67.467 | 54.052 | 1.00 | 0.00 |
| ATOM | 139 | CE1 | PHE | S | 13 | 20.760 | 69.375 | 52.487 | 1.00 | 0.00 |
| ATOM | 140 | CE2 | PHE | S | 13 | 20.752 | 67.564 | 54.154 | 1.00 | 0.00 |
| ATOM | 141 | CZ | PHE | S | 13 | 20.070 | 68.518 | 53.370 | 1.00 | 0.00 |
| ATOM | 142 | H | PHE | S | 13 | 26.275 | 65.637 | 52.031 | 1.00 | 0.00 |
| ATOM | 143 | N | ARG | S | 14 | 26.009 | 67.779 | 49.990 | 1.00 | 0.00 |
| ATOM | 144 | CA | ARG | S | 14 | 25.977 | 68.012 | 48.553 | 1.00 | 0.00 |
| ATOM | 145 | C | ARG | S | 14 | 25.576 | 66.762 | 47.825 | 1.00 | 0.00 |
| ATOM | 146 | O | ARG | S | 14 | 26.434 | 66.023 | 47.319 | 1.00 | 0.00 |
| ATOM | 147 | CB | ARG | S | 14 | 27.320 | 68.450 | 47.985 | 1.00 | 0.00 |
| ATOM | 148 | CG | ARG | S | 14 | 27.577 | 69.933 | 48.154 | 1.00 | 0.00 |
| ATOM | 149 | CD | ARG | S | 14 | 28.043 | 70.329 | 49.547 | 1.00 | 0.00 |
| ATOM | 150 | NE | ARG | S | 14 | 28.012 | 71.777 | 49.699 | 1.00 | 0.00 |
| ATOM | 151 | CZ | ARG | S | 14 | 29.002 | 72.564 | 49.230 | 1.00 | 0.00 |
| ATOM | 152 | NH1 | ARG | S | 14 | 28.917 | 73.873 | 49.437 | 1.00 | 0.00 |
| ATOM | 153 | NH2 | ARG | S | 14 | 30.051 | 72.084 | 48.559 | 1.00 | 0.00 |
| ATOM | 154 | H | ARG | S | 14 | 26.831 | 67.419 | 50.424 | 1.00 | 0.00 |
| ATOM | 155 | HE | ARG | S | 14 | 27.172 | 72.119 | 50.116 | 1.00 | 0.00 |
| ATOM | 156 | 1HH1 | ARG | S | 14 | 29.605 | 74.465 | 48.991 | 1.00 | 0.00 |
| ATOM | 157 | 2HH1 | ARG | S | 14 | 28.205 | 74.309 | 49.988 | 1.00 | 0.00 |
| ATOM | 158 | 1HH2 | ARG | S | 14 | 30.829 | 72.678 | 48.290 | 1.00 | 0.00 |
| ATOM | 159 | 2HH2 | ARG | S | 14 | 30.091 | 71.117 | 48.293 | 1.00 | 0.00 |
| ATOM | 160 | N | PHE | S | 15 | 24.253 | 66.582 | 47.813 | 1.00 | 0.00 |
| ATOM | 161 | CA | PHE | S | 15 | 23.685 | 65.410 | 47.168 | 1.00 | 0.00 |
| ATOM | 162 | C | PHE | S | 15 | 23.906 | 65.326 | 45.675 | 1.00 | 0.00 |
| ATOM | 163 | O | PHE | S | 15 | 23.092 | 65.748 | 44.855 | 1.00 | 0.00 |
| ATOM | 164 | CB | PHE | S | 15 | 22.204 | 65.253 | 47.518 | 1.00 | 0.00 |
| ATOM | 165 | CG | PHE | S | 15 | 21.995 | 65.130 | 49.011 | 1.00 | 0.00 |
| ATOM | 166 | CD1 | PHE | S | 15 | 21.049 | 65.972 | 49.633 | 1.00 | 0.00 |
| ATOM | 167 | CD2 | PHE | S | 15 | 22.725 | 64.177 | 49.757 | 1.00 | 0.00 |
| ATOM | 168 | CE1 | PHE | S | 15 | 20.821 | 65.851 | 51.016 | 1.00 | 0.00 |
| ATOM | 169 | CE2 | PHE | S | 15 | 22.501 | 64.056 | 51.141 | 1.00 | 0.00 |
| ATOM | 170 | CZ | PHE | S | 15 | 21.545 | 64.891 | 51.755 | 1.00 | 0.00 |
| ATOM | 171 | H | PHE | S | 15 | 23.696 | 67.227 | 48.338 | 1.00 | 0.00 |
| ATOM | 172 | N | GLY | S | 16 | 25.056 | 64.680 | 45.415 | 1.00 | 0.00 |
| ATOM | 173 | CA | GLY | S | 16 | 25.367 | 64.047 | 44.139 | 1.00 | 0.00 |
| ATOM | 174 | C | GLY | S | 16 | 24.880 | 62.609 | 44.164 | 1.00 | 0.00 |
| ATOM | 175 | O | GLY | S | 16 | 24.477 | 62.111 | 45.218 | 1.00 | 0.00 |
| ATOM | 176 | H | GLY | S | 16 | 25.570 | 64.494 | 46.248 | 1.00 | 0.00 |
| ATOM | 177 | N | THR | S | 17 | 24.874 | 62.013 | 42.955 | 1.00 | 0.00 |
| ATOM | 178 | CA | THR | S | 17 | 24.230 | 60.722 | 42.686 | 1.00 | 0.00 |
| ATOM | 179 | C | THR | S | 17 | 24.557 | 60.144 | 41.293 | 1.00 | 0.00 |
| ATOM | 180 | O | THR | S | 17 | 25.268 | 60.728 | 40.479 | 1.00 | 0.00 |
| ATOM | 181 | CB | THR | S | 17 | 22.708 | 60.831 | 42.981 | 1.00 | 0.00 |
| ATOM | 182 | OG1 | THR | S | 17 | 21.975 | 59.674 | 42.567 | 1.00 | 0.00 |
| ATOM | 183 | CG2 | THR | S | 17 | 22.052 | 62.064 | 42.384 | 1.00 | 0.00 |
| ATOM | 184 | H | THR | S | 17 | 25.440 | 62.364 | 42.210 | 1.00 | 0.00 |
| ATOM | 185 | HG1 | THR | S | 17 | 21.834 | 59.815 | 41.628 | 1.00 | 0.00 |
| ATOM | 186 | N | VAL | S | 18 | 24.008 | 58.926 | 41.081 | 1.00 | 0.00 |
| ATOM | 187 | CA | VAL | S | 18 | 24.028 | 58.089 | 39.868 | 1.00 | 0.00 |
| ATOM | 188 | C | VAL | S | 18 | 22.836 | 57.137 | 40.026 | 1.00 | 0.00 |
| ATOM | 189 | O | VAL | S | 18 | 22.102 | 57.326 | 40.990 | 1.00 | 0.00 |
| ATOM | 190 | CB | VAL | S | 18 | 25.359 | 57.312 | 39.754 | 1.00 | 0.00 |
| ATOM | 191 | CG1 | VAL | S | 18 | 26.355 | 58.076 | 38.907 | 1.00 | 0.00 |
| ATOM | 192 | CG2 | VAL | S | 18 | 25.977 | 56.901 | 41.091 | 1.00 | 0.00 |
| ATOM | 193 | H | VAL | S | 18 | 23.453 | 58.570 | 41.833 | 1.00 | 0.00 |
| ATOM | 194 | N | PRO | S | 19 | 22.628 | 56.111 | 39.146 | 1.00 | 0.00 |
| ATOM | 195 | CA | PRO | S | 19 | 21.998 | 54.873 | 39.634 | 1.00 | 0.00 |
| ATOM | 196 | C | PRO | S | 19 | 23.060 | 54.040 | 40.334 | 1.00 | 0.00 |
| ATOM | 197 | O | PRO | S | 19 | 24.173 | 54.508 | 40.549 | 1.00 | 0.00 |
| ATOM | 198 | CB | PRO | S | 19 | 21.561 | 54.201 | 38.332 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 199 | CG | PRO | S | 19 | 22.611 | 54.620 | 37.307 | 1.00 | 0.00 |
| ATOM | 200 | CD | PRO | S | 19 | 22.919 | 56.052 | 37.720 | 1.00 | 0.00 |
| ATOM | 201 | N | ASN | S | 20 | 22.739 | 52.777 | 40.630 | 1.00 | 0.00 |
| ATOM | 202 | CA | ASN | S | 20 | 23.896 | 51.907 | 40.864 | 1.00 | 0.00 |
| ATOM | 203 | C | ASN | S | 20 | 24.467 | 51.470 | 39.541 | 1.00 | 0.00 |
| ATOM | 204 | O | ASN | S | 20 | 24.047 | 50.440 | 39.019 | 1.00 | 0.00 |
| ATOM | 205 | CB | ASN | S | 20 | 23.549 | 50.663 | 41.696 | 1.00 | 0.00 |
| ATOM | 206 | CG | ASN | S | 20 | 23.956 | 50.899 | 43.132 | 1.00 | 0.00 |
| ATOM | 207 | OD1 | ASN | S | 20 | 24.140 | 52.039 | 43.556 | 1.00 | 0.00 |
| ATOM | 208 | ND2 | ASN | S | 20 | 24.123 | 49.802 | 43.861 | 1.00 | 0.00 |
| ATOM | 209 | H | ASN | S | 20 | 21.807 | 52.433 | 40.516 | 1.00 | 0.00 |
| ATOM | 210 | 1HD2 | ASN | S | 20 | 24.486 | 49.907 | 44.783 | 1.00 | 0.00 |
| ATOM | 211 | 2HD2 | ASN | S | 20 | 23.906 | 48.890 | 43.529 | 1.00 | 0.00 |
| ATOM | 212 | N | GLY | S | 21 | 25.370 | 52.313 | 39.020 | 1.00 | 0.00 |
| ATOM | 213 | CA | GLY | S | 21 | 25.862 | 52.113 | 37.661 | 1.00 | 0.00 |
| ATOM | 214 | C | GLY | S | 21 | 27.217 | 52.744 | 37.371 | 1.00 | 0.00 |
| ATOM | 215 | O | GLY | S | 21 | 28.204 | 52.474 | 38.053 | 1.00 | 0.00 |
| ATOM | 216 | H | GLY | S | 21 | 25.578 | 53.163 | 39.506 | 1.00 | 0.00 |
| ATOM | 217 | N | SER | S | 22 | 27.208 | 53.555 | 36.293 | 1.00 | 0.00 |
| ATOM | 218 | CA | SER | S | 22 | 28.422 | 53.834 | 35.519 | 1.00 | 0.00 |
| ATOM | 219 | C | SER | S | 22 | 29.610 | 54.536 | 36.193 | 1.00 | 0.00 |
| ATOM | 220 | O | SER | S | 22 | 30.735 | 54.039 | 36.177 | 1.00 | 0.00 |
| ATOM | 221 | CB | SER | S | 22 | 27.980 | 54.521 | 34.209 | 1.00 | 0.00 |
| ATOM | 222 | OG | SER | S | 22 | 28.876 | 54.228 | 33.121 | 1.00 | 0.00 |
| ATOM | 223 | H | SER | S | 22 | 26.347 | 53.787 | 35.838 | 1.00 | 0.00 |
| ATOM | 224 | HG | SER | S | 22 | 29.501 | 54.957 | 33.133 | 1.00 | 0.00 |
| ATOM | 225 | N | THR | S | 23 | 29.307 | 55.733 | 36.753 | 1.00 | 0.00 |
| ATOM | 226 | CA | THR | S | 23 | 30.399 | 56.659 | 37.092 | 1.00 | 0.00 |
| ATOM | 227 | C | THR | S | 23 | 30.577 | 57.102 | 38.549 | 1.00 | 0.00 |
| ATOM | 228 | O | THR | S | 23 | 31.575 | 56.734 | 39.163 | 1.00 | 0.00 |
| ATOM | 229 | CB | THR | S | 23 | 30.366 | 57.843 | 36.114 | 1.00 | 0.00 |
| ATOM | 230 | OG1 | THR | S | 23 | 30.836 | 57.422 | 34.826 | 1.00 | 0.00 |
| ATOM | 231 | CG2 | THR | S | 23 | 31.182 | 59.065 | 36.539 | 1.00 | 0.00 |
| ATOM | 232 | H | THR | S | 23 | 28.341 | 56.000 | 36.765 | 1.00 | 0.00 |
| ATOM | 233 | HG1 | THR | S | 23 | 30.363 | 56.637 | 34.539 | 1.00 | 0.00 |
| ATOM | 234 | N | GLU | S | 24 | 29.592 | 57.881 | 39.108 | 1.00 | 0.00 |
| ATOM | 235 | CA | GLU | S | 24 | 29.854 | 58.455 | 40.456 | 1.00 | 0.00 |
| ATOM | 236 | C | GLU | S | 24 | 30.387 | 57.440 | 41.460 | 1.00 | 0.00 |
| ATOM | 237 | O | GLU | S | 24 | 31.396 | 57.667 | 42.126 | 1.00 | 0.00 |
| ATOM | 238 | CB | GLU | S | 24 | 28.725 | 59.351 | 41.059 | 1.00 | 0.00 |
| ATOM | 239 | CG | GLU | S | 24 | 29.220 | 60.544 | 41.920 | 1.00 | 0.00 |
| ATOM | 240 | CD | GLU | S | 24 | 28.134 | 61.435 | 42.559 | 1.00 | 0.00 |
| ATOM | 241 | OE1 | GLU | S | 24 | 27.499 | 62.274 | 41.910 | 1.00 | 0.00 |
| ATOM | 242 | OE2 | GLU | S | 24 | 27.949 | 61.340 | 43.765 | 1.00 | 0.00 |
| ATOM | 243 | H | GLU | S | 24 | 28.890 | 58.254 | 38.497 | 1.00 | 0.00 |
| ATOM | 244 | N | ARG | S | 25 | 29.751 | 56.244 | 41.427 | 1.00 | 0.00 |
| ATOM | 245 | CA | ARG | S | 25 | 30.288 | 55.111 | 42.197 | 1.00 | 0.00 |
| ATOM | 246 | C | ARG | S | 25 | 31.808 | 54.889 | 42.143 | 1.00 | 0.00 |
| ATOM | 247 | O | ARG | S | 25 | 32.436 | 54.865 | 43.189 | 1.00 | 0.00 |
| ATOM | 248 | CB | ARG | S | 25 | 29.455 | 53.833 | 41.964 | 1.00 | 0.00 |
| ATOM | 249 | CG | ARG | S | 25 | 29.732 | 52.572 | 42.822 | 1.00 | 0.00 |
| ATOM | 250 | CD | ARG | S | 25 | 29.679 | 52.682 | 44.364 | 1.00 | 0.00 |
| ATOM | 251 | NE | ARG | S | 25 | 30.843 | 53.423 | 44.831 | 1.00 | 0.00 |
| ATOM | 252 | CZ | ARG | S | 25 | 30.794 | 54.388 | 45.773 | 1.00 | 0.00 |
| ATOM | 253 | NH1 | ARG | S | 25 | 31.545 | 55.459 | 45.597 | 1.00 | 0.00 |
| ATOM | 254 | NH2 | ARG | S | 25 | 30.016 | 54.305 | 46.851 | 1.00 | 0.00 |
| ATOM | 255 | H | ARG | S | 25 | 28.972 | 56.164 | 40.813 | 1.00 | 0.00 |
| ATOM | 256 | HE | ARG | S | 25 | 31.649 | 53.389 | 44.230 | 1.00 | 0.00 |
| ATOM | 257 | 1HH1 | ARG | S | 25 | 31.544 | 56.207 | 46.265 | 1.00 | 0.00 |
| ATOM | 258 | 2HH1 | ARG | S | 25 | 32.124 | 55.549 | 44.781 | 1.00 | 0.00 |
| ATOM | 259 | 1HH2 | ARG | S | 25 | 29.977 | 55.084 | 47.500 | 1.00 | 0.00 |
| ATOM | 260 | 2HH2 | ARG | S | 25 | 29.504 | 53.476 | 47.060 | 1.00 | 0.00 |
| ATOM | 261 | N | ASN | S | 26 | 32.415 | 54.826 | 40.947 | 1.00 | 0.00 |
| ATOM | 262 | CA | ASN | S | 26 | 33.893 | 54.856 | 41.009 | 1.00 | 0.00 |
| ATOM | 263 | C | ASN | S | 26 | 34.439 | 56.188 | 41.520 | 1.00 | 0.00 |
| ATOM | 264 | O | ASN | S | 26 | 35.011 | 56.280 | 42.608 | 1.00 | 0.00 |
| ATOM | 265 | CB | ASN | S | 26 | 34.546 | 54.460 | 39.670 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 266 | CG | ASN | S | 26 | 36.075 | 54.381 | 39.756 | 1.00 | 0.00 |
| ATOM | 267 | OD1 | ASN | S | 26 | 36.688 | 53.876 | 40.687 | 1.00 | 0.00 |
| ATOM | 268 | ND2 | ASN | S | 26 | 36.698 | 54.880 | 38.680 | 1.00 | 0.00 |
| ATOM | 269 | H | ASN | S | 26 | 31.920 | 54.923 | 40.083 | 1.00 | 0.00 |
| ATOM | 270 | 1HD2 | ASN | S | 26 | 37.694 | 54.869 | 38.586 | 1.00 | 0.00 |
| ATOM | 271 | 2HD2 | ASN | S | 26 | 36.192 | 55.317 | 37.929 | 1.00 | 0.00 |
| ATOM | 272 | N | ILE | S | 27 | 34.169 | 57.237 | 40.714 | 1.00 | 0.00 |
| ATOM | 273 | CA | ILE | S | 27 | 34.856 | 58.516 | 40.941 | 1.00 | 0.00 |
| ATOM | 274 | C | ILE | S | 27 | 34.916 | 58.979 | 42.378 | 1.00 | 0.00 |
| ATOM | 275 | O | ILE | S | 27 | 35.983 | 58.908 | 42.976 | 1.00 | 0.00 |
| ATOM | 276 | CB | ILE | S | 27 | 34.412 | 59.628 | 39.958 | 1.00 | 0.00 |
| ATOM | 277 | CG1 | ILE | S | 27 | 34.950 | 61.028 | 40.277 | 1.00 | 0.00 |
| ATOM | 278 | CG2 | ILE | S | 27 | 32.905 | 59.694 | 39.785 | 1.00 | 0.00 |
| ATOM | 279 | CD1 | ILE | S | 27 | 34.656 | 62.024 | 39.156 | 1.00 | 0.00 |
| ATOM | 280 | H | ILE | S | 27 | 33.576 | 57.073 | 39.926 | 1.00 | 0.00 |
| ATOM | 281 | N | ARG | S | 28 | 33.748 | 59.364 | 42.922 | 1.00 | 0.00 |
| ATOM | 282 | CA | ARG | S | 28 | 33.741 | 59.942 | 44.262 | 1.00 | 0.00 |
| ATOM | 283 | C | ARG | S | 28 | 34.169 | 59.019 | 45.391 | 1.00 | 0.00 |
| ATOM | 284 | O | ARG | S | 28 | 34.485 | 59.463 | 46.491 | 1.00 | 0.00 |
| ATOM | 285 | CB | ARG | S | 28 | 32.372 | 60.569 | 44.505 | 1.00 | 0.00 |
| ATOM | 286 | CG | ARG | S | 28 | 32.327 | 61.827 | 45.376 | 1.00 | 0.00 |
| ATOM | 287 | CD | ARG | S | 28 | 30.915 | 62.403 | 45.277 | 1.00 | 0.00 |
| ATOM | 288 | NE | ARG | S | 28 | 30.751 | 63.728 | 45.879 | 1.00 | 0.00 |
| ATOM | 289 | CZ | ARG | S | 28 | 29.493 | 64.215 | 45.990 | 1.00 | 0.00 |
| ATOM | 290 | NH1 | ARG | S | 28 | 29.253 | 65.379 | 46.589 | 1.00 | 0.00 |
| ATOM | 291 | NH2 | ARG | S | 28 | 28.469 | 63.524 | 45.490 | 1.00 | 0.00 |
| ATOM | 292 | H | ARG | S | 28 | 32.909 | 59.336 | 42.386 | 1.00 | 0.00 |
| ATOM | 293 | HE | ARG | S | 28 | 31.573 | 64.216 | 46.181 | 1.00 | 0.00 |
| ATOM | 294 | 1HH1 | ARG | S | 28 | 28.334 | 65.735 | 46.797 | 1.00 | 0.00 |
| ATOM | 295 | 2HH1 | ARG | S | 28 | 30.043 | 65.942 | 46.849 | 1.00 | 0.00 |
| ATOM | 296 | 1HH2 | ARG | S | 28 | 27.508 | 63.734 | 45.670 | 1.00 | 0.00 |
| ATOM | 297 | 2HH2 | ARG | S | 28 | 28.630 | 62.734 | 44.882 | 1.00 | 0.00 |
| ATOM | 298 | N | ASN | S | 29 | 34.176 | 57.709 | 45.084 | 1.00 | 0.00 |
| ATOM | 299 | CA | ASN | S | 29 | 34.803 | 56.758 | 46.017 | 1.00 | 0.00 |
| ATOM | 300 | C | ASN | S | 29 | 36.263 | 57.087 | 46.224 | 1.00 | 0.00 |
| ATOM | 301 | O | ASN | S | 29 | 36.725 | 57.490 | 47.287 | 1.00 | 0.00 |
| ATOM | 302 | CB | ASN | S | 29 | 34.720 | 55.310 | 45.509 | 1.00 | 0.00 |
| ATOM | 303 | CG | ASN | S | 29 | 34.669 | 54.318 | 46.651 | 1.00 | 0.00 |
| ATOM | 304 | OD1 | ASN | S | 29 | 33.679 | 54.262 | 47.371 | 1.00 | 0.00 |
| ATOM | 305 | ND2 | ASN | S | 29 | 35.723 | 53.511 | 46.750 | 1.00 | 0.00 |
| ATOM | 306 | H | ASN | S | 29 | 33.936 | 57.456 | 44.152 | 1.00 | 0.00 |
| ATOM | 307 | 1HD2 | ASN | S | 29 | 35.758 | 52.838 | 47.486 | 1.00 | 0.00 |
| ATOM | 308 | 2HD2 | ASN | S | 29 | 36.439 | 53.560 | 46.053 | 1.00 | 0.00 |
| ATOM | 309 | N | ASN | S | 30 | 36.988 | 56.936 | 45.113 | 1.00 | 0.00 |
| ATOM | 310 | CA | ASN | S | 30 | 38.398 | 57.327 | 45.120 | 1.00 | 0.00 |
| ATOM | 311 | C | ASN | S | 30 | 38.613 | 58.804 | 45.443 | 1.00 | 0.00 |
| ATOM | 312 | O | ASN | S | 30 | 39.524 | 59.200 | 46.152 | 1.00 | 0.00 |
| ATOM | 313 | CB | ASN | S | 30 | 39.048 | 56.915 | 43.796 | 1.00 | 0.00 |
| ATOM | 314 | CG | ASN | S | 30 | 40.558 | 56.873 | 43.936 | 1.00 | 0.00 |
| ATOM | 315 | OD1 | ASN | S | 30 | 41.290 | 57.810 | 43.645 | 1.00 | 0.00 |
| ATOM | 316 | ND2 | ASN | S | 30 | 41.016 | 55.706 | 44.409 | 1.00 | 0.00 |
| ATOM | 317 | H | ASN | S | 30 | 36.533 | 56.601 | 44.292 | 1.00 | 0.00 |
| ATOM | 318 | 1HD2 | ASN | S | 30 | 42.001 | 55.549 | 44.506 | 1.00 | 0.00 |
| ATOM | 319 | 2HD2 | ASN | S | 30 | 40.392 | 54.974 | 44.686 | 1.00 | 0.00 |
| ATOM | 320 | N | TYR | S | 31 | 37.660 | 59.600 | 44.957 | 1.00 | 0.00 |
| ATOM | 321 | CA | TYR | S | 31 | 37.669 | 61.050 | 45.108 | 1.00 | 0.00 |
| ATOM | 322 | C | TYR | S | 31 | 36.956 | 61.472 | 46.376 | 1.00 | 0.00 |
| ATOM | 323 | O | TYR | S | 31 | 36.161 | 62.412 | 46.365 | 1.00 | 0.00 |
| ATOM | 324 | CB | TYR | S | 31 | 36.941 | 61.672 | 43.915 | 1.00 | 0.00 |
| ATOM | 325 | CG | TYR | S | 31 | 37.620 | 62.900 | 43.372 | 1.00 | 0.00 |
| ATOM | 326 | CD1 | TYR | S | 31 | 38.066 | 62.849 | 42.040 | 1.00 | 0.00 |
| ATOM | 327 | CD2 | TYR | S | 31 | 37.775 | 64.049 | 44.176 | 1.00 | 0.00 |
| ATOM | 328 | CE1 | TYR | S | 31 | 38.692 | 63.973 | 41.492 | 1.00 | 0.00 |
| ATOM | 329 | CE2 | TYR | S | 31 | 38.401 | 65.178 | 43.627 | 1.00 | 0.00 |
| ATOM | 330 | CZ | TYR | S | 31 | 38.851 | 65.117 | 42.293 | 1.00 | 0.00 |
| ATOM | 331 | OH | TYR | S | 31 | 39.479 | 66.208 | 41.731 | 1.00 | 0.00 |
| ATOM | 332 | H | TYR | S | 31 | 36.861 | 59.148 | 44.577 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 333 | HH | TYR | S | 31 | 39.688 | 66.855 | 42.401 | 1.00 | 0.00 |
| ATOM | 334 | N | ALA | S | 32 | 37.235 | 60.706 | 47.453 | 1.00 | 0.00 |
| ATOM | 335 | CA | ALA | S | 32 | 36.629 | 60.868 | 48.782 | 1.00 | 0.00 |
| ATOM | 336 | C | ALA | S | 32 | 35.110 | 60.918 | 48.806 | 1.00 | 0.00 |
| ATOM | 337 | O | ALA | S | 32 | 34.490 | 61.806 | 48.222 | 1.00 | 0.00 |
| ATOM | 338 | CB | ALA | S | 32 | 37.180 | 62.107 | 49.495 | 1.00 | 0.00 |
| ATOM | 339 | H | ALA | S | 32 | 37.940 | 60.002 | 47.347 | 1.00 | 0.00 |
| ATOM | 340 | N | GLU | S | 33 | 34.514 | 59.929 | 49.496 | 1.00 | 0.00 |
| ATOM | 341 | CA | GLU | S | 33 | 33.054 | 59.971 | 49.549 | 1.00 | 0.00 |
| ATOM | 342 | C | GLU | S | 33 | 32.496 | 60.963 | 50.557 | 1.00 | 0.00 |
| ATOM | 343 | O | GLU | S | 33 | 32.077 | 60.676 | 51.675 | 1.00 | 0.00 |
| ATOM | 344 | CB | GLU | S | 33 | 32.411 | 58.575 | 49.615 | 1.00 | 0.00 |
| ATOM | 345 | CG | GLU | S | 33 | 30.908 | 58.642 | 49.289 | 1.00 | 0.00 |
| ATOM | 346 | CD | GLU | S | 33 | 30.355 | 57.310 | 48.803 | 1.00 | 0.00 |
| ATOM | 347 | OE1 | GLU | S | 33 | 29.337 | 56.853 | 49.316 | 1.00 | 0.00 |
| ATOM | 348 | OE2 | GLU | S | 33 | 30.909 | 56.730 | 47.876 | 1.00 | 0.00 |
| ATOM | 349 | H | GLU | S | 33 | 35.076 | 59.217 | 49.915 | 1.00 | 0.00 |
| ATOM | 350 | N | MET | S | 34 | 32.513 | 62.198 | 50.046 | 1.00 | 0.00 |
| ATOM | 351 | CA | MET | S | 34 | 31.760 | 63.353 | 50.504 | 1.00 | 0.00 |
| ATOM | 352 | C | MET | S | 34 | 30.304 | 62.939 | 50.501 | 1.00 | 0.00 |
| ATOM | 353 | O | MET | S | 34 | 29.672 | 62.925 | 49.450 | 1.00 | 0.00 |
| ATOM | 354 | CB | MET | S | 34 | 32.106 | 64.404 | 49.443 | 1.00 | 0.00 |
| ATOM | 355 | CG | MET | S | 34 | 31.279 | 65.672 | 49.241 | 1.00 | 0.00 |
| ATOM | 356 | SD | MET | S | 34 | 31.960 | 66.555 | 47.819 | 1.00 | 0.00 |
| ATOM | 357 | CE | MET | S | 34 | 31.004 | 68.077 | 47.899 | 1.00 | 0.00 |
| ATOM | 358 | H | MET | S | 34 | 33.000 | 62.259 | 49.179 | 1.00 | 0.00 |
| ATOM | 359 | N | HIS | S | 35 | 29.838 | 62.514 | 51.684 | 1.00 | 0.00 |
| ATOM | 360 | CA | HIS | S | 35 | 28.544 | 61.829 | 51.749 | 1.00 | 0.00 |
| ATOM | 361 | C | HIS | S | 35 | 27.442 | 62.485 | 50.928 | 1.00 | 0.00 |
| ATOM | 362 | O | HIS | S | 35 | 27.149 | 63.671 | 51.046 | 1.00 | 0.00 |
| ATOM | 363 | CB | HIS | S | 35 | 28.139 | 61.628 | 53.218 | 1.00 | 0.00 |
| ATOM | 364 | CG | HIS | S | 35 | 26.715 | 61.133 | 53.323 | 1.00 | 0.00 |
| ATOM | 365 | ND1 | HIS | S | 35 | 26.331 | 59.864 | 53.090 | 1.00 | 0.00 |
| ATOM | 366 | CD2 | HIS | S | 35 | 25.588 | 61.900 | 53.628 | 1.00 | 0.00 |
| ATOM | 367 | CE1 | HIS | S | 35 | 24.970 | 59.822 | 53.244 | 1.00 | 0.00 |
| ATOM | 368 | NE2 | HIS | S | 35 | 24.515 | 61.078 | 53.572 | 1.00 | 0.00 |
| ATOM | 369 | H | HIS | S | 35 | 30.490 | 62.439 | 52.441 | 1.00 | 0.00 |
| ATOM | 370 | HD1 | HIS | S | 35 | 26.906 | 59.101 | 52.864 | 1.00 | 0.00 |
| ATOM | 371 | N | ALA | S | 36 | 26.871 | 61.653 | 50.061 | 1.00 | 0.00 |
| ATOM | 372 | CA | ALA | S | 36 | 25.825 | 62.151 | 49.180 | 1.00 | 0.00 |
| ATOM | 373 | C | ALA | S | 36 | 24.777 | 61.087 | 48.948 | 1.00 | 0.00 |
| ATOM | 374 | O | ALA | S | 36 | 24.901 | 59.963 | 49.435 | 1.00 | 0.00 |
| ATOM | 375 | CB | ALA | S | 36 | 26.440 | 62.550 | 47.845 | 1.00 | 0.00 |
| ATOM | 376 | H | ALA | S | 36 | 27.151 | 60.693 | 50.060 | 1.00 | 0.00 |
| ATOM | 377 | N | TYR | S | 37 | 23.766 | 61.465 | 48.144 | 1.00 | 0.00 |
| ATOM | 378 | CA | TYR | S | 37 | 22.724 | 60.500 | 47.781 | 1.00 | 0.00 |
| ATOM | 379 | C | TYR | S | 37 | 23.148 | 59.631 | 46.596 | 1.00 | 0.00 |
| ATOM | 380 | O | TYR | S | 37 | 22.405 | 59.347 | 45.662 | 1.00 | 0.00 |
| ATOM | 381 | CB | TYR | S | 37 | 21.420 | 61.289 | 47.536 | 1.00 | 0.00 |
| ATOM | 382 | CG | TYR | S | 37 | 20.115 | 60.501 | 47.530 | 1.00 | 0.00 |
| ATOM | 383 | CD1 | TYR | S | 37 | 18.934 | 61.209 | 47.842 | 1.00 | 0.00 |
| ATOM | 384 | CD2 | TYR | S | 37 | 20.066 | 59.135 | 47.173 | 1.00 | 0.00 |
| ATOM | 385 | CE1 | TYR | S | 37 | 17.686 | 60.583 | 47.674 | 1.00 | 0.00 |
| ATOM | 386 | CE2 | TYR | S | 37 | 18.824 | 58.509 | 46.989 | 1.00 | 0.00 |
| ATOM | 387 | CZ | TYR | S | 37 | 17.650 | 59.259 | 47.190 | 1.00 | 0.00 |
| ATOM | 388 | OH | TYR | S | 37 | 16.436 | 58.678 | 46.863 | 1.00 | 0.00 |
| ATOM | 389 | H | TYR | S | 37 | 23.798 | 62.358 | 47.701 | 1.00 | 0.00 |
| ATOM | 390 | HH | TYR | S | 37 | 15.752 | 59.051 | 47.415 | 1.00 | 0.00 |
| ATOM | 391 | N | MET | S | 38 | 24.414 | 59.207 | 46.681 | 1.00 | 0.00 |
| ATOM | 392 | CA | MET | S | 38 | 25.010 | 58.455 | 45.589 | 1.00 | 0.00 |
| ATOM | 393 | C | MET | S | 38 | 24.245 | 57.183 | 45.296 | 1.00 | 0.00 |
| ATOM | 394 | O | MET | S | 38 | 23.695 | 56.520 | 46.185 | 1.00 | 0.00 |
| ATOM | 395 | CB | MET | S | 38 | 26.475 | 58.176 | 45.898 | 1.00 | 0.00 |
| ATOM | 396 | CG | MET | S | 38 | 27.283 | 57.815 | 44.653 | 1.00 | 0.00 |
| ATOM | 397 | SD | MET | S | 38 | 28.985 | 57.453 | 45.066 | 1.00 | 0.00 |
| ATOM | 398 | CE | MET | S | 38 | 29.343 | 59.022 | 45.866 | 1.00 | 0.00 |
| ATOM | 399 | H | MET | S | 38 | 24.946 | 59.407 | 47.499 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 400 | N | GLY | S | 39 | 24.195 | 56.911 | 43.999 | 1.00 | 0.00 |
| ATOM | 401 | CA | GLY | S | 39 | 23.184 | 56.061 | 43.388 | 1.00 | 0.00 |
| ATOM | 402 | C | GLY | S | 39 | 22.824 | 54.737 | 44.003 | 1.00 | 0.00 |
| ATOM | 403 | O | GLY | S | 39 | 23.444 | 54.238 | 44.942 | 1.00 | 0.00 |
| ATOM | 404 | H | GLY | S | 39 | 24.833 | 57.436 | 43.441 | 1.00 | 0.00 |
| ATOM | 405 | N | LYS | S | 40 | 21.722 | 54.225 | 43.430 | 1.00 | 0.00 |
| ATOM | 406 | CA | LYS | S | 40 | 21.147 | 52.912 | 43.743 | 1.00 | 0.00 |
| ATOM | 407 | C | LYS | S | 40 | 20.192 | 52.472 | 42.649 | 1.00 | 0.00 |
| ATOM | 408 | O | LYS | S | 40 | 20.391 | 51.510 | 41.912 | 1.00 | 0.00 |
| ATOM | 409 | CB | LYS | S | 40 | 20.425 | 52.929 | 45.093 | 1.00 | 0.00 |
| ATOM | 410 | CG | LYS | S | 40 | 21.219 | 52.237 | 46.200 | 1.00 | 0.00 |
| ATOM | 411 | CD | LYS | S | 40 | 20.853 | 52.782 | 47.583 | 1.00 | 0.00 |
| ATOM | 412 | CE | LYS | S | 40 | 21.115 | 54.289 | 47.692 | 1.00 | 0.00 |
| ATOM | 413 | NZ | LYS | S | 40 | 22.522 | 54.568 | 47.403 | 1.00 | 0.00 |
| ATOM | 414 | H | LYS | S | 40 | 21.367 | 54.796 | 42.684 | 1.00 | 0.00 |
| ATOM | 415 | 1HZ | LYS | S | 40 | 23.132 | 54.180 | 48.136 | 1.00 | 0.00 |
| ATOM | 416 | 2HZ | LYS | S | 40 | 22.782 | 54.150 | 46.489 | 1.00 | 0.00 |
| ATOM | 417 | 3HZ | LYS | S | 40 | 22.688 | 55.586 | 47.317 | 1.00 | 0.00 |
| ATOM | 418 | N | PHE | S | 41 | 19.117 | 53.259 | 42.585 | 1.00 | 0.00 |
| ATOM | 419 | CA | PHE | S | 41 | 18.236 | 53.146 | 41.432 | 1.00 | 0.00 |
| ATOM | 420 | C | PHE | S | 41 | 18.330 | 54.473 | 40.726 | 1.00 | 0.00 |
| ATOM | 421 | O | PHE | S | 41 | 18.772 | 55.456 | 41.317 | 1.00 | 0.00 |
| ATOM | 422 | CB | PHE | S | 41 | 16.796 | 52.869 | 41.873 | 1.00 | 0.00 |
| ATOM | 423 | CG | PHE | S | 41 | 16.723 | 51.550 | 42.608 | 1.00 | 0.00 |
| ATOM | 424 | CD1 | PHE | S | 41 | 16.634 | 51.549 | 44.017 | 1.00 | 0.00 |
| ATOM | 425 | CD2 | PHE | S | 41 | 16.753 | 50.342 | 41.876 | 1.00 | 0.00 |
| ATOM | 426 | CE1 | PHE | S | 41 | 16.585 | 50.323 | 44.707 | 1.00 | 0.00 |
| ATOM | 427 | CE2 | PHE | S | 41 | 16.704 | 49.115 | 42.565 | 1.00 | 0.00 |
| ATOM | 428 | CZ | PHE | S | 41 | 16.623 | 49.118 | 43.974 | 1.00 | 0.00 |
| ATOM | 429 | H | PHE | S | 41 | 19.031 | 54.092 | 43.132 | 1.00 | 0.00 |
| ATOM | 430 | N | ASN | S | 42 | 17.937 | 54.489 | 39.447 | 1.00 | 0.00 |
| ATOM | 431 | CA | ASN | S | 42 | 17.922 | 55.835 | 38.870 | 1.00 | 0.00 |
| ATOM | 432 | C | ASN | S | 42 | 16.532 | 56.395 | 38.761 | 1.00 | 0.00 |
| ATOM | 433 | O | ASN | S | 42 | 16.301 | 57.508 | 38.334 | 1.00 | 0.00 |
| ATOM | 434 | CB | ASN | S | 42 | 18.598 | 55.937 | 37.510 | 1.00 | 0.00 |
| ATOM | 435 | CG | ASN | S | 42 | 18.961 | 57.391 | 37.260 | 1.00 | 0.00 |
| ATOM | 436 | OD1 | ASN | S | 42 | 19.220 | 58.191 | 38.163 | 1.00 | 0.00 |
| ATOM | 437 | ND2 | ASN | S | 42 | 19.023 | 57.705 | 35.969 | 1.00 | 0.00 |
| ATOM | 438 | H | ASN | S | 42 | 17.492 | 53.689 | 39.037 | 1.00 | 0.00 |
| ATOM | 439 | 1HD2 | ASN | S | 42 | 19.488 | 58.547 | 35.687 | 1.00 | 0.00 |
| ATOM | 440 | 2HD2 | ASN | S | 42 | 18.602 | 57.115 | 35.286 | 1.00 | 0.00 |
| ATOM | 441 | N | GLN | S | 43 | 15.580 | 55.561 | 39.183 | 1.00 | 0.00 |
| ATOM | 442 | CA | GLN | S | 43 | 14.201 | 56.000 | 39.004 | 1.00 | 0.00 |
| ATOM | 443 | C | GLN | S | 43 | 13.874 | 57.157 | 39.943 | 1.00 | 0.00 |
| ATOM | 444 | O | GLN | S | 43 | 13.472 | 58.236 | 39.532 | 1.00 | 0.00 |
| ATOM | 445 | CB | GLN | S | 43 | 13.290 | 54.771 | 39.142 | 1.00 | 0.00 |
| ATOM | 446 | CG | GLN | S | 43 | 13.337 | 53.768 | 37.963 | 1.00 | 0.00 |
| ATOM | 447 | CD | GLN | S | 43 | 14.709 | 53.132 | 37.725 | 1.00 | 0.00 |
| ATOM | 448 | OE1 | GLN | S | 43 | 15.521 | 52.928 | 38.626 | 1.00 | 0.00 |
| ATOM | 449 | NE2 | GLN | S | 43 | 14.961 | 52.860 | 36.440 | 1.00 | 0.00 |
| ATOM | 450 | H | GLN | S | 43 | 15.765 | 54.636 | 39.516 | 1.00 | 0.00 |
| ATOM | 451 | 1HE2 | GLN | S | 43 | 15.869 | 52.531 | 36.172 | 1.00 | 0.00 |
| ATOM | 452 | 2HE2 | GLN | S | 43 | 14.264 | 52.973 | 35.734 | 1.00 | 0.00 |
| ATOM | 453 | N | ARG | S | 44 | 14.185 | 56.883 | 41.231 | 1.00 | 0.00 |
| ATOM | 454 | CA | ARG | S | 44 | 14.220 | 57.979 | 42.212 | 1.00 | 0.00 |
| ATOM | 455 | C | ARG | S | 44 | 15.401 | 58.924 | 42.040 | 1.00 | 0.00 |
| ATOM | 456 | O | ARG | S | 44 | 15.439 | 60.051 | 42.534 | 1.00 | 0.00 |
| ATOM | 457 | CB | ARG | S | 44 | 14.190 | 57.434 | 43.643 | 1.00 | 0.00 |
| ATOM | 458 | CG | ARG | S | 44 | 12.848 | 56.824 | 44.065 | 1.00 | 0.00 |
| ATOM | 459 | CD | ARG | S | 44 | 11.728 | 57.855 | 44.254 | 1.00 | 0.00 |
| ATOM | 460 | NE | ARG | S | 44 | 10.474 | 57.199 | 44.620 | 1.00 | 0.00 |
| ATOM | 461 | CZ | ARG | S | 44 | 9.290 | 57.530 | 44.041 | 1.00 | 0.00 |
| ATOM | 462 | NH1 | ARG | S | 44 | 8.178 | 56.927 | 44.469 | 1.00 | 0.00 |
| ATOM | 463 | NH2 | ARG | S | 44 | 9.194 | 58.415 | 43.056 | 1.00 | 0.00 |
| ATOM | 464 | H | ARG | S | 44 | 14.567 | 55.985 | 41.426 | 1.00 | 0.00 |
| ATOM | 465 | HE | ARG | S | 44 | 10.504 | 56.529 | 45.362 | 1.00 | 0.00 |
| ATOM | 466 | 1HH1 | ARG | S | 44 | 7.292 | 57.135 | 44.051 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 467 | 2HH1 | ARG | S | 44 | 8.191 | 56.249 | 45.206 | 1.00 | 0.00 |
| ATOM | 468 | 1HH2 | ARG | S | 44 | 8.341 | 58.780 | 42.683 | 1.00 | 0.00 |
| ATOM | 469 | 2HH2 | ARG | S | 44 | 10.017 | 58.778 | 42.598 | 1.00 | 0.00 |
| ATOM | 470 | N | GLY | S | 45 | 16.382 | 58.404 | 41.279 | 1.00 | 0.00 |
| ATOM | 471 | CA | GLY | S | 45 | 17.380 | 59.317 | 40.735 | 1.00 | 0.00 |
| ATOM | 472 | C | GLY | S | 45 | 16.747 | 60.431 | 39.924 | 1.00 | 0.00 |
| ATOM | 473 | O | GLY | S | 45 | 17.057 | 61.597 | 40.130 | 1.00 | 0.00 |
| ATOM | 474 | H | GLY | S | 45 | 16.348 | 57.440 | 41.037 | 1.00 | 0.00 |
| ATOM | 475 | N | VAL | S | 46 | 15.829 | 60.035 | 39.032 | 1.00 | 0.00 |
| ATOM | 476 | CA | VAL | S | 46 | 15.150 | 60.995 | 38.163 | 1.00 | 0.00 |
| ATOM | 477 | C | VAL | S | 46 | 14.159 | 61.864 | 38.911 | 1.00 | 0.00 |
| ATOM | 478 | O | VAL | S | 46 | 14.122 | 63.074 | 38.720 | 1.00 | 0.00 |
| ATOM | 479 | CB | VAL | S | 46 | 14.493 | 60.298 | 36.956 | 1.00 | 0.00 |
| ATOM | 480 | CG1 | VAL | S | 46 | 13.732 | 61.271 | 36.047 | 1.00 | 0.00 |
| ATOM | 481 | CG2 | VAL | S | 46 | 15.534 | 59.534 | 36.138 | 1.00 | 0.00 |
| ATOM | 482 | H | VAL | S | 46 | 15.535 | 59.082 | 39.015 | 1.00 | 0.00 |
| ATOM | 483 | N | ASP | S | 47 | 13.392 | 61.245 | 39.831 | 1.00 | 0.00 |
| ATOM | 484 | CA | ASP | S | 47 | 12.411 | 62.048 | 40.587 | 1.00 | 0.00 |
| ATOM | 485 | C | ASP | S | 47 | 12.978 | 63.340 | 41.157 | 1.00 | 0.00 |
| ATOM | 486 | O | ASP | S | 47 | 12.491 | 64.449 | 40.984 | 1.00 | 0.00 |
| ATOM | 487 | CB | ASP | S | 47 | 11.827 | 61.279 | 41.774 | 1.00 | 0.00 |
| ATOM | 488 | CG | ASP | S | 47 | 10.947 | 60.124 | 41.357 | 1.00 | 0.00 |
| ATOM | 489 | OD1 | ASP | S | 47 | 11.402 | 58.984 | 41.409 | 1.00 | 0.00 |
| ATOM | 490 | OD2 | ASP | S | 47 | 9.779 | 60.335 | 41.045 | 1.00 | 0.00 |
| ATOM | 491 | H | ASP | S | 47 | 13.373 | 60.244 | 39.919 | 1.00 | 0.00 |
| ATOM | 492 | N | ASP | S | 48 | 14.109 | 63.161 | 41.848 | 1.00 | 0.00 |
| ATOM | 493 | CA | ASP | S | 48 | 14.615 | 64.338 | 42.561 | 1.00 | 0.00 |
| ATOM | 494 | C | ASP | S | 48 | 15.392 | 65.359 | 41.750 | 1.00 | 0.00 |
| ATOM | 495 | O | ASP | S | 48 | 16.005 | 66.279 | 42.298 | 1.00 | 0.00 |
| ATOM | 496 | CB | ASP | S | 48 | 15.478 | 64.017 | 43.777 | 1.00 | 0.00 |
| ATOM | 497 | CG | ASP | S | 48 | 14.946 | 62.968 | 44.734 | 1.00 | 0.00 |
| ATOM | 498 | OD1 | ASP | S | 48 | 15.398 | 62.957 | 45.869 | 1.00 | 0.00 |
| ATOM | 499 | OD2 | ASP | S | 48 | 14.171 | 62.096 | 44.360 | 1.00 | 0.00 |
| ATOM | 500 | H | ASP | S | 48 | 14.550 | 62.266 | 41.920 | 1.00 | 0.00 |
| ATOM | 501 | N | ALA | S | 49 | 15.341 | 65.195 | 40.423 | 1.00 | 0.00 |
| ATOM | 502 | CA | ALA | S | 49 | 15.638 | 66.376 | 39.632 | 1.00 | 0.00 |
| ATOM | 503 | C | ALA | S | 49 | 14.405 | 67.264 | 39.542 | 1.00 | 0.00 |
| ATOM | 504 | O | ALA | S | 49 | 14.470 | 68.477 | 39.717 | 1.00 | 0.00 |
| ATOM | 505 | CB | ALA | S | 49 | 16.146 | 65.979 | 38.250 | 1.00 | 0.00 |
| ATOM | 506 | H | ALA | S | 49 | 14.877 | 64.416 | 40.004 | 1.00 | 0.00 |
| ATOM | 507 | N | LEU | S | 50 | 13.251 | 66.609 | 39.349 | 1.00 | 0.00 |
| ATOM | 508 | CA | LEU | S | 50 | 11.961 | 67.293 | 39.494 | 1.00 | 0.00 |
| ATOM | 509 | C | LEU | S | 50 | 11.730 | 67.902 | 40.880 | 1.00 | 0.00 |
| ATOM | 510 | O | LEU | S | 50 | 11.120 | 68.955 | 41.050 | 1.00 | 0.00 |
| ATOM | 511 | CB | LEU | S | 50 | 10.830 | 66.336 | 39.085 | 1.00 | 0.00 |
| ATOM | 512 | CG | LEU | S | 50 | 9.393 | 66.834 | 39.288 | 1.00 | 0.00 |
| ATOM | 513 | CD1 | LEU | S | 50 | 9.070 | 68.085 | 38.470 | 1.00 | 0.00 |
| ATOM | 514 | CD2 | LEU | S | 50 | 8.382 | 65.713 | 39.052 | 1.00 | 0.00 |
| ATOM | 515 | H | LEU | S | 50 | 13.327 | 65.615 | 39.249 | 1.00 | 0.00 |
| ATOM | 516 | N | LEU | S | 51 | 12.268 | 67.200 | 41.880 | 1.00 | 0.00 |
| ATOM | 517 | CA | LEU | S | 51 | 12.269 | 67.783 | 43.222 | 1.00 | 0.00 |
| ATOM | 518 | C | LEU | S | 51 | 13.443 | 68.725 | 43.478 | 1.00 | 0.00 |
| ATOM | 519 | O | LEU | S | 51 | 13.441 | 69.570 | 44.366 | 1.00 | 0.00 |
| ATOM | 520 | CB | LEU | S | 51 | 12.199 | 66.650 | 44.250 | 1.00 | 0.00 |
| ATOM | 521 | CG | LEU | S | 51 | 11.837 | 67.074 | 45.676 | 1.00 | 0.00 |
| ATOM | 522 | CD1 | LEU | S | 51 | 10.499 | 67.814 | 45.740 | 1.00 | 0.00 |
| ATOM | 523 | CD2 | LEU | S | 51 | 11.870 | 65.882 | 46.633 | 1.00 | 0.00 |
| ATOM | 524 | H | LEU | S | 51 | 12.729 | 66.340 | 41.659 | 1.00 | 0.00 |
| ATOM | 525 | N | SER | S | 52 | 14.478 | 68.527 | 42.646 | 1.00 | 0.00 |
| ATOM | 526 | CA | SER | S | 52 | 15.717 | 69.293 | 42.802 | 1.00 | 0.00 |
| ATOM | 527 | C | SER | S | 52 | 16.382 | 69.163 | 44.172 | 1.00 | 0.00 |
| ATOM | 528 | O | SER | S | 52 | 17.100 | 70.044 | 44.650 | 1.00 | 0.00 |
| ATOM | 529 | CB | SER | S | 52 | 15.470 | 70.751 | 42.408 | 1.00 | 0.00 |
| ATOM | 530 | OG | SER | S | 52 | 15.104 | 70.830 | 41.013 | 1.00 | 0.00 |
| ATOM | 531 | H | SER | S | 52 | 14.428 | 67.786 | 41.985 | 1.00 | 0.00 |
| ATOM | 532 | HG | SER | S | 52 | 14.497 | 70.087 | 40.888 | 1.00 | 0.00 |
| ATOM | 533 | N | LEU | S | 53 | 16.083 | 68.021 | 44.818 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 534 | CA | LEU | S | 53 | 16.553 | 67.819 | 46.192 | 1.00 | 0.00 |
| ATOM | 535 | C | LEU | S | 53 | 18.029 | 67.472 | 46.265 | 1.00 | 0.00 |
| ATOM | 536 | O | LEU | S | 53 | 18.837 | 68.116 | 46.948 | 1.00 | 0.00 |
| ATOM | 537 | CB | LEU | S | 53 | 15.699 | 66.743 | 46.871 | 1.00 | 0.00 |
| ATOM | 538 | CG | LEU | S | 53 | 15.991 | 66.537 | 48.361 | 1.00 | 0.00 |
| ATOM | 539 | CD1 | LEU | S | 53 | 15.662 | 67.780 | 49.190 | 1.00 | 0.00 |
| ATOM | 540 | CD2 | LEU | S | 53 | 15.300 | 65.284 | 48.900 | 1.00 | 0.00 |
| ATOM | 541 | H | LEU | S | 53 | 15.589 | 67.288 | 44.348 | 1.00 | 0.00 |
| ATOM | 542 | N | LYS | S | 54 | 18.313 | 66.431 | 45.473 | 1.00 | 0.00 |
| ATOM | 543 | CA | LYS | S | 54 | 19.682 | 66.104 | 45.123 | 1.00 | 0.00 |
| ATOM | 544 | C | LYS | S | 54 | 20.319 | 67.291 | 44.410 | 1.00 | 0.00 |
| ATOM | 545 | O | LYS | S | 54 | 20.060 | 67.528 | 43.240 | 1.00 | 0.00 |
| ATOM | 546 | CB | LYS | S | 54 | 19.668 | 64.861 | 44.217 | 1.00 | 0.00 |
| ATOM | 547 | CG | LYS | S | 54 | 18.994 | 63.600 | 44.794 | 1.00 | 0.00 |
| ATOM | 548 | CD | LYS | S | 54 | 18.793 | 62.522 | 43.713 | 1.00 | 0.00 |
| ATOM | 549 | CE | LYS | S | 54 | 18.314 | 61.130 | 44.162 | 1.00 | 0.00 |
| ATOM | 550 | NZ | LYS | S | 54 | 16.869 | 61.052 | 44.445 | 1.00 | 0.00 |
| ATOM | 551 | H | LYS | S | 54 | 17.539 | 66.003 | 45.018 | 1.00 | 0.00 |
| ATOM | 552 | 1HZ | LYS | S | 54 | 16.591 | 60.099 | 44.730 | 1.00 | 0.00 |
| ATOM | 553 | 2HZ | LYS | S | 54 | 16.534 | 61.695 | 45.196 | 1.00 | 0.00 |
| ATOM | 554 | 3HZ | LYS | S | 54 | 16.270 | 61.258 | 43.615 | 1.00 | 0.00 |
| ATOM | 555 | N | THR | S | 55 | 21.154 | 68.054 | 45.143 | 1.00 | 0.00 |
| ATOM | 556 | CA | THR | S | 55 | 21.900 | 69.109 | 44.435 | 1.00 | 0.00 |
| ATOM | 557 | C | THR | S | 55 | 23.157 | 68.599 | 43.719 | 1.00 | 0.00 |
| ATOM | 558 | O | THR | S | 55 | 24.316 | 68.847 | 44.086 | 1.00 | 0.00 |
| ATOM | 559 | CB | THR | S | 55 | 22.158 | 70.341 | 45.347 | 1.00 | 0.00 |
| ATOM | 560 | OG1 | THR | S | 55 | 22.798 | 71.421 | 44.631 | 1.00 | 0.00 |
| ATOM | 561 | CG2 | THR | S | 55 | 22.921 | 69.995 | 46.632 | 1.00 | 0.00 |
| ATOM | 562 | H | THR | S | 55 | 21.237 | 67.900 | 46.125 | 1.00 | 0.00 |
| ATOM | 563 | HG1 | THR | S | 55 | 22.301 | 71.475 | 43.816 | 1.00 | 0.00 |
| ATOM | 564 | N | GLY | S | 56 | 22.849 | 67.854 | 42.645 | 1.00 | 0.00 |
| ATOM | 565 | CA | GLY | S | 56 | 23.861 | 67.238 | 41.787 | 1.00 | 0.00 |
| ATOM | 566 | C | GLY | S | 56 | 23.654 | 65.761 | 41.468 | 1.00 | 0.00 |
| ATOM | 567 | O | GLY | S | 56 | 23.102 | 64.986 | 42.238 | 1.00 | 0.00 |
| ATOM | 568 | H | GLY | S | 56 | 21.885 | 67.815 | 42.381 | 1.00 | 0.00 |
| ATOM | 569 | N | LYS | S | 57 | 24.181 | 65.342 | 40.299 | 1.00 | 0.00 |
| ATOM | 570 | CA | LYS | S | 57 | 24.323 | 63.907 | 39.974 | 1.00 | 0.00 |
| ATOM | 571 | C | LYS | S | 57 | 25.505 | 63.741 | 39.028 | 1.00 | 0.00 |
| ATOM | 572 | O | LYS | S | 57 | 25.544 | 64.573 | 38.140 | 1.00 | 0.00 |
| ATOM | 573 | CB | LYS | S | 57 | 23.013 | 63.463 | 39.290 | 1.00 | 0.00 |
| ATOM | 574 | CG | LYS | S | 57 | 22.955 | 62.029 | 38.748 | 1.00 | 0.00 |
| ATOM | 575 | CD | LYS | S | 57 | 21.593 | 61.603 | 38.192 | 1.00 | 0.00 |
| ATOM | 576 | CE | LYS | S | 57 | 21.683 | 60.349 | 37.310 | 1.00 | 0.00 |
| ATOM | 577 | NZ | LYS | S | 57 | 22.463 | 60.650 | 36.106 | 1.00 | 0.00 |
| ATOM | 578 | H | LYS | S | 57 | 24.285 | 66.058 | 39.594 | 1.00 | 0.00 |
| ATOM | 579 | 1HZ | LYS | S | 57 | 23.284 | 60.017 | 36.018 | 1.00 | 0.00 |
| ATOM | 580 | 2HZ | LYS | S | 57 | 21.844 | 60.581 | 35.269 | 1.00 | 0.00 |
| ATOM | 581 | 3HZ | LYS | S | 57 | 22.787 | 61.640 | 36.153 | 1.00 | 0.00 |
| ATOM | 582 | N | LEU | S | 58 | 26.418 | 62.755 | 39.185 | 1.00 | 0.00 |
| ATOM | 583 | CA | LEU | S | 58 | 27.307 | 62.451 | 38.044 | 1.00 | 0.00 |
| ATOM | 584 | C | LEU | S | 58 | 26.672 | 61.398 | 37.128 | 1.00 | 0.00 |
| ATOM | 585 | O | LEU | S | 58 | 25.442 | 61.397 | 37.071 | 1.00 | 0.00 |
| ATOM | 586 | CB | LEU | S | 58 | 28.728 | 62.092 | 38.502 | 1.00 | 0.00 |
| ATOM | 587 | CG | LEU | S | 58 | 29.527 | 63.214 | 39.175 | 1.00 | 0.00 |
| ATOM | 588 | CD1 | LEU | S | 58 | 30.911 | 62.736 | 39.587 | 1.00 | 0.00 |
| ATOM | 589 | CD2 | LEU | S | 58 | 29.671 | 64.467 | 38.322 | 1.00 | 0.00 |
| ATOM | 590 | H | LEU | S | 58 | 26.401 | 62.136 | 39.972 | 1.00 | 0.00 |
| ATOM | 591 | N | ASP | S | 59 | 27.456 | 60.539 | 36.447 | 1.00 | 0.00 |
| ATOM | 592 | CA | ASP | S | 59 | 27.147 | 59.601 | 35.341 | 1.00 | 0.00 |
| ATOM | 593 | C | ASP | S | 59 | 28.002 | 60.068 | 34.175 | 1.00 | 0.00 |
| ATOM | 594 | O | ASP | S | 59 | 29.071 | 60.606 | 34.468 | 1.00 | 0.00 |
| ATOM | 595 | CB | ASP | S | 59 | 25.672 | 59.314 | 34.957 | 1.00 | 0.00 |
| ATOM | 596 | CG | ASP | S | 59 | 25.018 | 58.282 | 35.881 | 1.00 | 0.00 |
| ATOM | 597 | OD1 | ASP | S | 59 | 24.241 | 58.668 | 36.736 | 1.00 | 0.00 |
| ATOM | 598 | OD2 | ASP | S | 59 | 25.249 | 57.077 | 35.785 | 1.00 | 0.00 |
| ATOM | 599 | H | ASP | S | 59 | 28.423 | 60.615 | 36.663 | 1.00 | 0.00 |
| ATOM | 600 | N | ALA | S | 60 | 27.614 | 59.852 | 32.905 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 601 | CA | ALA | S | 60 | 28.577 | 60.231 | 31.869 | 1.00 | 0.00 |
| ATOM | 602 | C | ALA | S | 60 | 27.935 | 60.744 | 30.598 | 1.00 | 0.00 |
| ATOM | 603 | O | ALA | S | 60 | 27.353 | 59.980 | 29.824 | 1.00 | 0.00 |
| ATOM | 604 | CB | ALA | S | 60 | 29.494 | 59.054 | 31.518 | 1.00 | 0.00 |
| ATOM | 605 | H | ALA | S | 60 | 26.689 | 59.608 | 32.606 | 1.00 | 0.00 |
| ATOM | 606 | N | PHE | S | 61 | 28.085 | 62.069 | 30.427 | 1.00 | 0.00 |
| ATOM | 607 | CA | PHE | S | 61 | 27.480 | 62.778 | 29.295 | 1.00 | 0.00 |
| ATOM | 608 | C | PHE | S | 61 | 25.986 | 62.535 | 29.062 | 1.00 | 0.00 |
| ATOM | 609 | O | PHE | S | 61 | 25.203 | 62.789 | 29.972 | 1.00 | 0.00 |
| ATOM | 610 | CB | PHE | S | 61 | 28.372 | 62.704 | 28.047 | 1.00 | 0.00 |
| ATOM | 611 | CG | PHE | S | 61 | 28.919 | 64.084 | 27.753 | 1.00 | 0.00 |
| ATOM | 612 | CD1 | PHE | S | 61 | 30.070 | 64.536 | 28.434 | 1.00 | 0.00 |
| ATOM | 613 | CD2 | PHE | S | 61 | 28.272 | 64.902 | 26.801 | 1.00 | 0.00 |
| ATOM | 614 | CE1 | PHE | S | 61 | 30.590 | 65.814 | 28.149 | 1.00 | 0.00 |
| ATOM | 615 | CE2 | PHE | S | 61 | 28.788 | 66.181 | 26.515 | 1.00 | 0.00 |
| ATOM | 616 | CZ | PHE | S | 61 | 29.946 | 66.622 | 27.189 | 1.00 | 0.00 |
| ATOM | 617 | H | PHE | S | 61 | 28.680 | 62.518 | 31.091 | 1.00 | 0.00 |
| ATOM | 618 | N | ILE | S | 62 | 25.583 | 62.066 | 27.853 | 1.00 | 0.00 |
| ATOM | 619 | CA | ILE | S | 62 | 24.149 | 62.070 | 27.463 | 1.00 | 0.00 |
| ATOM | 620 | C | ILE | S | 62 | 23.109 | 61.650 | 28.516 | 1.00 | 0.00 |
| ATOM | 621 | O | ILE | S | 62 | 22.069 | 62.275 | 28.753 | 1.00 | 0.00 |
| ATOM | 622 | CB | ILE | S | 62 | 23.988 | 61.303 | 26.130 | 1.00 | 0.00 |
| ATOM | 623 | CG1 | ILE | S | 62 | 22.561 | 61.336 | 25.576 | 1.00 | 0.00 |
| ATOM | 624 | CG2 | ILE | S | 62 | 24.513 | 59.861 | 26.222 | 1.00 | 0.00 |
| ATOM | 625 | CD1 | ILE | S | 62 | 22.452 | 60.748 | 24.167 | 1.00 | 0.00 |
| ATOM | 626 | H | ILE | S | 62 | 26.266 | 61.798 | 27.175 | 1.00 | 0.00 |
| ATOM | 627 | N | TYR | S | 63 | 23.518 | 60.572 | 29.226 | 1.00 | 0.00 |
| ATOM | 628 | CA | TYR | S | 63 | 22.726 | 59.955 | 30.303 | 1.00 | 0.00 |
| ATOM | 629 | C | TYR | S | 63 | 22.093 | 60.894 | 31.311 | 1.00 | 0.00 |
| ATOM | 630 | O | TYR | S | 63 | 21.001 | 60.662 | 31.837 | 1.00 | 0.00 |
| ATOM | 631 | CB | TYR | S | 63 | 23.527 | 58.875 | 31.044 | 1.00 | 0.00 |
| ATOM | 632 | CG | TYR | S | 63 | 24.154 | 57.918 | 30.058 | 1.00 | 0.00 |
| ATOM | 633 | CD1 | TYR | S | 63 | 23.350 | 57.294 | 29.082 | 1.00 | 0.00 |
| ATOM | 634 | CD2 | TYR | S | 63 | 25.544 | 57.702 | 30.131 | 1.00 | 0.00 |
| ATOM | 635 | CE1 | TYR | S | 63 | 23.967 | 56.503 | 28.104 | 1.00 | 0.00 |
| ATOM | 636 | CE2 | TYR | S | 63 | 26.163 | 56.909 | 29.153 | 1.00 | 0.00 |
| ATOM | 637 | CZ | TYR | S | 63 | 25.367 | 56.345 | 28.138 | 1.00 | 0.00 |
| ATOM | 638 | OH | TYR | S | 63 | 25.970 | 55.612 | 27.132 | 1.00 | 0.00 |
| ATOM | 639 | H | TYR | S | 63 | 24.354 | 60.141 | 28.898 | 1.00 | 0.00 |
| ATOM | 640 | HH | TYR | S | 63 | 25.307 | 55.485 | 26.447 | 1.00 | 0.00 |
| ATOM | 641 | N | ASP | S | 64 | 22.788 | 62.014 | 31.540 | 1.00 | 0.00 |
| ATOM | 642 | CA | ASP | S | 64 | 22.055 | 63.172 | 32.047 | 1.00 | 0.00 |
| ATOM | 643 | C | ASP | S | 64 | 21.959 | 64.295 | 31.039 | 1.00 | 0.00 |
| ATOM | 644 | O | ASP | S | 64 | 20.877 | 64.736 | 30.670 | 1.00 | 0.00 |
| ATOM | 645 | CB | ASP | S | 64 | 22.646 | 63.766 | 33.328 | 1.00 | 0.00 |
| ATOM | 646 | CG | ASP | S | 64 | 22.127 | 63.143 | 34.610 | 1.00 | 0.00 |
| ATOM | 647 | OD1 | ASP | S | 64 | 21.208 | 62.349 | 34.584 | 1.00 | 0.00 |
| ATOM | 648 | OD2 | ASP | S | 64 | 22.634 | 63.434 | 35.683 | 1.00 | 0.00 |
| ATOM | 649 | H | ASP | S | 64 | 23.709 | 62.099 | 31.162 | 1.00 | 0.00 |
| ATOM | 650 | N | ALA | S | 65 | 23.150 | 64.784 | 30.648 | 1.00 | 0.00 |
| ATOM | 651 | CA | ALA | S | 65 | 23.274 | 66.129 | 30.071 | 1.00 | 0.00 |
| ATOM | 652 | C | ALA | S | 65 | 22.147 | 66.572 | 29.157 | 1.00 | 0.00 |
| ATOM | 653 | O | ALA | S | 65 | 21.497 | 67.608 | 29.361 | 1.00 | 0.00 |
| ATOM | 654 | CB | ALA | S | 65 | 24.597 | 66.257 | 29.313 | 1.00 | 0.00 |
| ATOM | 655 | H | ALA | S | 65 | 23.948 | 64.230 | 30.879 | 1.00 | 0.00 |
| ATOM | 656 | N | ALA | S | 66 | 21.973 | 65.695 | 28.154 | 1.00 | 0.00 |
| ATOM | 657 | CA | ALA | S | 66 | 20.917 | 65.881 | 27.171 | 1.00 | 0.00 |
| ATOM | 658 | C | ALA | S | 66 | 19.528 | 65.478 | 27.642 | 1.00 | 0.00 |
| ATOM | 659 | O | ALA | S | 66 | 18.645 | 66.325 | 27.773 | 1.00 | 0.00 |
| ATOM | 660 | CB | ALA | S | 66 | 21.257 | 65.137 | 25.877 | 1.00 | 0.00 |
| ATOM | 661 | H | ALA | S | 66 | 22.446 | 64.820 | 28.230 | 1.00 | 0.00 |
| ATOM | 662 | N | VAL | S | 67 | 19.324 | 64.175 | 27.868 | 1.00 | 0.00 |
| ATOM | 663 | CA | VAL | S | 67 | 17.963 | 63.640 | 28.041 | 1.00 | 0.00 |
| ATOM | 664 | C | VAL | S | 67 | 17.238 | 63.999 | 29.350 | 1.00 | 0.00 |
| ATOM | 665 | O | VAL | S | 67 | 16.011 | 63.968 | 29.498 | 1.00 | 0.00 |
| ATOM | 666 | CB | VAL | S | 67 | 18.000 | 62.110 | 27.831 | 1.00 | 0.00 |
| ATOM | 667 | CG1 | VAL | S | 67 | 16.608 | 61.473 | 27.759 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 668 | CG2 | VAL | S | 67 | 18.812 | 61.744 | 26.585 | 1.00 | 0.00 |
| ATOM | 669 | H | VAL | S | 67 | 20.155 | 63.628 | 27.954 | 1.00 | 0.00 |
| ATOM | 670 | N | LEU | S | 68 | 18.059 | 64.289 | 30.363 | 1.00 | 0.00 |
| ATOM | 671 | CA | LEU | S | 68 | 17.502 | 64.343 | 31.715 | 1.00 | 0.00 |
| ATOM | 672 | C | LEU | S | 68 | 16.778 | 65.602 | 32.168 | 1.00 | 0.00 |
| ATOM | 673 | O | LEU | S | 68 | 17.357 | 66.641 | 32.494 | 1.00 | 0.00 |
| ATOM | 674 | CB | LEU | S | 68 | 18.546 | 63.971 | 32.771 | 1.00 | 0.00 |
| ATOM | 675 | CG | LEU | S | 68 | 17.926 | 63.569 | 34.115 | 1.00 | 0.00 |
| ATOM | 676 | CD1 | LEU | S | 68 | 17.782 | 62.054 | 34.239 | 1.00 | 0.00 |
| ATOM | 677 | CD2 | LEU | S | 68 | 18.632 | 64.213 | 35.311 | 1.00 | 0.00 |
| ATOM | 678 | H | LEU | S | 68 | 19.036 | 64.405 | 30.174 | 1.00 | 0.00 |
| ATOM | 679 | N | ASN | S | 69 | 15.462 | 65.380 | 32.317 | 1.00 | 0.00 |
| ATOM | 680 | CA | ASN | S | 69 | 14.682 | 66.115 | 33.324 | 1.00 | 0.00 |
| ATOM | 681 | C | ASN | S | 69 | 14.860 | 67.624 | 33.338 | 1.00 | 0.00 |
| ATOM | 682 | O | ASN | S | 69 | 15.334 | 68.265 | 34.281 | 1.00 | 0.00 |
| ATOM | 683 | CB | ASN | S | 69 | 14.876 | 65.517 | 34.732 | 1.00 | 0.00 |
| ATOM | 684 | CG | ASN | S | 69 | 13.834 | 66.011 | 35.731 | 1.00 | 0.00 |
| ATOM | 685 | OD1 | ASN | S | 69 | 13.564 | 67.199 | 35.901 | 1.00 | 0.00 |
| ATOM | 686 | ND2 | ASN | S | 69 | 13.209 | 65.034 | 36.392 | 1.00 | 0.00 |
| ATOM | 687 | H | ASN | S | 69 | 15.146 | 64.582 | 31.811 | 1.00 | 0.00 |
| ATOM | 688 | 1HD2 | ASN | S | 69 | 12.450 | 65.212 | 37.013 | 1.00 | 0.00 |
| ATOM | 689 | 2HD2 | ASN | S | 69 | 13.581 | 64.108 | 36.326 | 1.00 | 0.00 |
| ATOM | 690 | N | TYR | S | 70 | 14.378 | 68.202 | 32.239 | 1.00 | 0.00 |
| ATOM | 691 | CA | TYR | S | 70 | 14.141 | 69.635 | 32.371 | 1.00 | 0.00 |
| ATOM | 692 | C | TYR | S | 70 | 12.721 | 69.935 | 32.812 | 1.00 | 0.00 |
| ATOM | 693 | O | TYR | S | 70 | 12.062 | 70.864 | 32.365 | 1.00 | 0.00 |
| ATOM | 694 | CB | TYR | S | 70 | 14.584 | 70.352 | 31.092 | 1.00 | 0.00 |
| ATOM | 695 | CG | TYR | S | 70 | 16.089 | 70.220 | 31.019 | 1.00 | 0.00 |
| ATOM | 696 | CD1 | TYR | S | 70 | 16.673 | 69.238 | 30.189 | 1.00 | 0.00 |
| ATOM | 697 | CD2 | TYR | S | 70 | 16.867 | 71.064 | 31.834 | 1.00 | 0.00 |
| ATOM | 698 | CE1 | TYR | S | 70 | 18.067 | 69.050 | 30.233 | 1.00 | 0.00 |
| ATOM | 699 | CE2 | TYR | S | 70 | 18.254 | 70.874 | 31.876 | 1.00 | 0.00 |
| ATOM | 700 | CZ | TYR | S | 70 | 18.835 | 69.854 | 31.100 | 1.00 | 0.00 |
| ATOM | 701 | OH | TYR | S | 70 | 20.197 | 69.643 | 31.221 | 1.00 | 0.00 |
| ATOM | 702 | H | TYR | S | 70 | 14.068 | 67.633 | 31.477 | 1.00 | 0.00 |
| ATOM | 703 | HH | TYR | S | 70 | 20.444 | 68.870 | 30.702 | 1.00 | 0.00 |
| ATOM | 704 | N | MET | S | 71 | 12.241 | 69.060 | 33.705 | 1.00 | 0.00 |
| ATOM | 705 | CA | MET | S | 71 | 10.856 | 69.121 | 34.148 | 1.00 | 0.00 |
| ATOM | 706 | C | MET | S | 71 | 10.677 | 70.140 | 35.251 | 1.00 | 0.00 |
| ATOM | 707 | O | MET | S | 71 | 9.840 | 71.035 | 35.182 | 1.00 | 0.00 |
| ATOM | 708 | CB | MET | S | 71 | 10.379 | 67.727 | 34.565 | 1.00 | 0.00 |
| ATOM | 709 | CG | MET | S | 71 | 8.861 | 67.631 | 34.722 | 1.00 | 0.00 |
| ATOM | 710 | SD | MET | S | 71 | 8.328 | 66.008 | 35.290 | 1.00 | 0.00 |
| ATOM | 711 | CE | MET | S | 71 | 6.563 | 66.344 | 35.392 | 1.00 | 0.00 |
| ATOM | 712 | H | MET | S | 71 | 12.832 | 68.372 | 34.117 | 1.00 | 0.00 |
| ATOM | 713 | N | ALA | S | 72 | 11.564 | 70.041 | 36.250 | 1.00 | 0.00 |
| ATOM | 714 | CA | ALA | S | 72 | 11.576 | 71.110 | 37.255 | 1.00 | 0.00 |
| ATOM | 715 | C | ALA | S | 72 | 12.294 | 72.393 | 36.872 | 1.00 | 0.00 |
| ATOM | 716 | O | ALA | S | 72 | 13.016 | 73.001 | 37.667 | 1.00 | 0.00 |
| ATOM | 717 | CB | ALA | S | 72 | 12.153 | 70.650 | 38.587 | 1.00 | 0.00 |
| ATOM | 718 | H | ALA | S | 72 | 12.193 | 69.266 | 36.226 | 1.00 | 0.00 |
| ATOM | 719 | N | GLY | S | 73 | 12.027 | 72.817 | 35.638 | 1.00 | 0.00 |
| ATOM | 720 | CA | GLY | S | 73 | 12.465 | 74.143 | 35.240 | 1.00 | 0.00 |
| ATOM | 721 | C | GLY | S | 73 | 13.332 | 74.124 | 34.008 | 1.00 | 0.00 |
| ATOM | 722 | O | GLY | S | 73 | 13.088 | 73.418 | 33.034 | 1.00 | 0.00 |
| ATOM | 723 | H | GLY | S | 73 | 11.478 | 72.274 | 35.007 | 1.00 | 0.00 |
| ATOM | 724 | N | ARG | S | 74 | 14.360 | 74.974 | 34.123 | 1.00 | 0.00 |
| ATOM | 725 | CA | ARG | S | 74 | 15.378 | 75.000 | 33.083 | 1.00 | 0.00 |
| ATOM | 726 | C | ARG | S | 74 | 16.643 | 74.283 | 33.537 | 1.00 | 0.00 |
| ATOM | 727 | O | ARG | S | 74 | 17.587 | 74.129 | 32.781 | 1.00 | 0.00 |
| ATOM | 728 | CB | ARG | S | 74 | 15.704 | 76.460 | 32.711 | 1.00 | 0.00 |
| ATOM | 729 | CG | ARG | S | 74 | 16.665 | 76.621 | 31.522 | 1.00 | 0.00 |
| ATOM | 730 | CD | ARG | S | 74 | 17.615 | 77.816 | 31.652 | 1.00 | 0.00 |
| ATOM | 731 | NE | ARG | S | 74 | 18.925 | 77.500 | 31.074 | 1.00 | 0.00 |
| ATOM | 732 | CZ | ARG | S | 74 | 19.247 | 77.803 | 29.796 | 1.00 | 0.00 |
| ATOM | 733 | NH1 | ARG | S | 74 | 20.434 | 77.440 | 29.332 | 1.00 | 0.00 |
| ATOM | 734 | NH2 | ARG | S | 74 | 18.386 | 78.434 | 28.999 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 735 | H | ARG | S | 74 | 14.551 | 75.395 | 35.010 | 1.00 | 0.00 |
| ATOM | 736 | HE | ARG | S | 74 | 19.579 | 76.970 | 31.639 | 1.00 | 0.00 |
| ATOM | 737 | 1HH1 | ARG | S | 74 | 20.687 | 77.543 | 28.370 | 1.00 | 0.00 |
| ATOM | 738 | 2HH1 | ARG | S | 74 | 21.110 | 77.038 | 29.959 | 1.00 | 0.00 |
| ATOM | 739 | 1HH2 | ARG | S | 74 | 18.627 | 78.668 | 28.056 | 1.00 | 0.00 |
| ATOM | 740 | 2HH2 | ARG | S | 74 | 17.483 | 78.683 | 29.338 | 1.00 | 0.00 |
| ATOM | 741 | N | ASP | S | 75 | 16.667 | 73.917 | 34.830 | 1.00 | 0.00 |
| ATOM | 742 | CA | ASP | S | 75 | 17.996 | 73.731 | 35.425 | 1.00 | 0.00 |
| ATOM | 743 | C | ASP | S | 75 | 18.868 | 72.543 | 34.998 | 1.00 | 0.00 |
| ATOM | 744 | O | ASP | S | 75 | 18.728 | 71.397 | 35.452 | 1.00 | 0.00 |
| ATOM | 745 | CB | ASP | S | 75 | 17.930 | 73.795 | 36.949 | 1.00 | 0.00 |
| ATOM | 746 | CG | ASP | S | 75 | 17.104 | 74.936 | 37.506 | 1.00 | 0.00 |
| ATOM | 747 | OD1 | ASP | S | 75 | 17.639 | 75.989 | 37.840 | 1.00 | 0.00 |
| ATOM | 748 | OD2 | ASP | S | 75 | 15.904 | 74.759 | 37.654 | 1.00 | 0.00 |
| ATOM | 749 | H | ASP | S | 75 | 15.904 | 74.095 | 35.449 | 1.00 | 0.00 |
| ATOM | 750 | N | GLU | S | 76 | 19.790 | 72.922 | 34.096 | 1.00 | 0.00 |
| ATOM | 751 | CA | GLU | S | 76 | 20.919 | 72.104 | 33.667 | 1.00 | 0.00 |
| ATOM | 752 | C | GLU | S | 76 | 21.994 | 71.991 | 34.732 | 1.00 | 0.00 |
| ATOM | 753 | O | GLU | S | 76 | 22.141 | 70.971 | 35.395 | 1.00 | 0.00 |
| ATOM | 754 | CB | GLU | S | 76 | 21.541 | 72.604 | 32.343 | 1.00 | 0.00 |
| ATOM | 755 | CG | GLU | S | 76 | 20.833 | 73.731 | 31.566 | 1.00 | 0.00 |
| ATOM | 756 | CD | GLU | S | 76 | 21.155 | 75.124 | 32.105 | 1.00 | 0.00 |
| ATOM | 757 | OE1 | GLU | S | 76 | 20.994 | 75.399 | 33.288 | 1.00 | 0.00 |
| ATOM | 758 | OE2 | GLU | S | 76 | 21.553 | 75.980 | 31.326 | 1.00 | 0.00 |
| ATOM | 759 | H | GLU | S | 76 | 19.692 | 73.855 | 33.751 | 1.00 | 0.00 |
| ATOM | 760 | N | GLY | S | 77 | 22.752 | 73.085 | 34.878 | 1.00 | 0.00 |
| ATOM | 761 | CA | GLY | S | 77 | 23.709 | 73.150 | 35.985 | 1.00 | 0.00 |
| ATOM | 762 | C | GLY | S | 77 | 24.952 | 72.335 | 35.766 | 1.00 | 0.00 |
| ATOM | 763 | O | GLY | S | 77 | 25.123 | 71.235 | 36.279 | 1.00 | 0.00 |
| ATOM | 764 | H | GLY | S | 77 | 22.522 | 73.883 | 34.318 | 1.00 | 0.00 |
| ATOM | 765 | N | CYS | S | 78 | 25.796 | 72.913 | 34.922 | 1.00 | 0.00 |
| ATOM | 766 | CA | CYS | S | 78 | 27.074 | 72.263 | 34.645 | 1.00 | 0.00 |
| ATOM | 767 | C | CYS | S | 78 | 28.198 | 73.047 | 35.301 | 1.00 | 0.00 |
| ATOM | 768 | O | CYS | S | 78 | 27.910 | 74.017 | 36.006 | 1.00 | 0.00 |
| ATOM | 769 | CB | CYS | S | 78 | 27.254 | 72.184 | 33.133 | 1.00 | 0.00 |
| ATOM | 770 | SG | CYS | S | 78 | 25.766 | 71.558 | 32.307 | 1.00 | 0.00 |
| ATOM | 771 | H | CYS | S | 78 | 25.629 | 73.849 | 34.633 | 1.00 | 0.00 |
| ATOM | 772 | N | LYS | S | 79 | 29.454 | 72.664 | 34.976 | 1.00 | 0.00 |
| ATOM | 773 | CA | LYS | S | 79 | 30.691 | 73.416 | 35.270 | 1.00 | 0.00 |
| ATOM | 774 | C | LYS | S | 79 | 31.413 | 72.872 | 36.491 | 1.00 | 0.00 |
| ATOM | 775 | O | LYS | S | 79 | 31.303 | 73.321 | 37.638 | 1.00 | 0.00 |
| ATOM | 776 | CB | LYS | S | 79 | 30.491 | 74.948 | 35.231 | 1.00 | 0.00 |
| ATOM | 777 | CG | LYS | S | 79 | 31.526 | 75.894 | 35.835 | 1.00 | 0.00 |
| ATOM | 778 | CD | LYS | S | 79 | 30.985 | 77.325 | 35.753 | 1.00 | 0.00 |
| ATOM | 779 | CE | LYS | S | 79 | 31.629 | 78.290 | 36.748 | 1.00 | 0.00 |
| ATOM | 780 | NZ | LYS | S | 79 | 31.324 | 77.841 | 38.110 | 1.00 | 0.00 |
| ATOM | 781 | H | LYS | S | 79 | 29.486 | 71.697 | 34.738 | 1.00 | 0.00 |
| ATOM | 782 | 1HZ | LYS | S | 79 | 31.656 | 76.874 | 38.257 | 1.00 | 0.00 |
| ATOM | 783 | 2HZ | LYS | S | 79 | 31.752 | 78.465 | 38.816 | 1.00 | 0.00 |
| ATOM | 784 | 3HZ | LYS | S | 79 | 30.300 | 77.804 | 38.274 | 1.00 | 0.00 |
| ATOM | 785 | N | LEU | S | 80 | 32.146 | 71.813 | 36.109 | 1.00 | 0.00 |
| ATOM | 786 | CA | LEU | S | 80 | 32.530 | 70.704 | 36.971 | 1.00 | 0.00 |
| ATOM | 787 | C | LEU | S | 80 | 33.643 | 70.988 | 37.959 | 1.00 | 0.00 |
| ATOM | 788 | O | LEU | S | 80 | 34.730 | 70.432 | 37.901 | 1.00 | 0.00 |
| ATOM | 789 | CB | LEU | S | 80 | 32.828 | 69.531 | 36.039 | 1.00 | 0.00 |
| ATOM | 790 | CG | LEU | S | 80 | 32.710 | 68.132 | 36.631 | 1.00 | 0.00 |
| ATOM | 791 | CD1 | LEU | S | 80 | 31.386 | 67.909 | 37.361 | 1.00 | 0.00 |
| ATOM | 792 | CD2 | LEU | S | 80 | 32.929 | 67.095 | 35.532 | 1.00 | 0.00 |
| ATOM | 793 | H | LEU | S | 80 | 32.381 | 71.742 | 35.139 | 1.00 | 0.00 |
| ATOM | 794 | N | VAL | S | 81 | 33.263 | 71.875 | 38.903 | 1.00 | 0.00 |
| ATOM | 795 | CA | VAL | S | 81 | 34.214 | 72.605 | 39.758 | 1.00 | 0.00 |
| ATOM | 796 | C | VAL | S | 81 | 35.477 | 71.875 | 40.184 | 1.00 | 0.00 |
| ATOM | 797 | O | VAL | S | 81 | 36.559 | 72.444 | 40.204 | 1.00 | 0.00 |
| ATOM | 798 | CB | VAL | S | 81 | 33.493 | 73.223 | 40.977 | 1.00 | 0.00 |
| ATOM | 799 | CG1 | VAL | S | 81 | 34.420 | 73.921 | 41.982 | 1.00 | 0.00 |
| ATOM | 800 | CG2 | VAL | S | 81 | 32.428 | 74.211 | 40.516 | 1.00 | 0.00 |
| ATOM | 801 | H | VAL | S | 81 | 32.301 | 72.135 | 38.809 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 802 | N | THR | S | 82 | 35.316 | 70.602 | 40.530 | 1.00 | 0.00 |
| ATOM | 803 | CA | THR | S | 82 | 36.520 | 69.896 | 40.963 | 1.00 | 0.00 |
| ATOM | 804 | C | THR | S | 82 | 36.522 | 68.488 | 40.430 | 1.00 | 0.00 |
| ATOM | 805 | O | THR | S | 82 | 37.449 | 67.995 | 39.802 | 1.00 | 0.00 |
| ATOM | 806 | CB | THR | S | 82 | 36.551 | 69.865 | 42.491 | 1.00 | 0.00 |
| ATOM | 807 | OG1 | THR | S | 82 | 35.195 | 69.785 | 42.964 | 1.00 | 0.00 |
| ATOM | 808 | CG2 | THR | S | 82 | 37.257 | 71.072 | 43.114 | 1.00 | 0.00 |
| ATOM | 809 | H | THR | S | 82 | 34.439 | 70.147 | 40.388 | 1.00 | 0.00 |
| ATOM | 810 | HG1 | THR | S | 82 | 35.263 | 69.861 | 43.917 | 1.00 | 0.00 |
| ATOM | 811 | N | ILE | S | 83 | 35.389 | 67.857 | 40.774 | 1.00 | 0.00 |
| ATOM | 812 | CA | ILE | S | 83 | 35.343 | 66.406 | 40.820 | 1.00 | 0.00 |
| ATOM | 813 | C | ILE | S | 83 | 35.730 | 65.690 | 39.539 | 1.00 | 0.00 |
| ATOM | 814 | O | ILE | S | 83 | 36.363 | 64.644 | 39.563 | 1.00 | 0.00 |
| ATOM | 815 | CB | ILE | S | 83 | 33.985 | 65.979 | 41.398 | 1.00 | 0.00 |
| ATOM | 816 | CG1 | ILE | S | 83 | 34.001 | 64.545 | 41.913 | 1.00 | 0.00 |
| ATOM | 817 | CG2 | ILE | S | 83 | 32.836 | 66.206 | 40.406 | 1.00 | 0.00 |
| ATOM | 818 | CD1 | ILE | S | 83 | 32.680 | 64.200 | 42.590 | 1.00 | 0.00 |
| ATOM | 819 | H | ILE | S | 83 | 34.656 | 68.393 | 41.182 | 1.00 | 0.00 |
| ATOM | 820 | N | GLY | S | 84 | 35.364 | 66.293 | 38.402 | 1.00 | 0.00 |
| ATOM | 821 | CA | GLY | S | 84 | 35.698 | 65.580 | 37.168 | 1.00 | 0.00 |
| ATOM | 822 | C | GLY | S | 84 | 37.077 | 65.861 | 36.606 | 1.00 | 0.00 |
| ATOM | 823 | O | GLY | S | 84 | 37.524 | 65.245 | 35.643 | 1.00 | 0.00 |
| ATOM | 824 | H | GLY | S | 84 | 35.002 | 67.223 | 38.430 | 1.00 | 0.00 |
| ATOM | 825 | N | SER | S | 85 | 37.754 | 66.831 | 37.224 | 1.00 | 0.00 |
| ATOM | 826 | CA | SER | S | 85 | 39.103 | 67.088 | 36.741 | 1.00 | 0.00 |
| ATOM | 827 | C | SER | S | 85 | 40.196 | 66.206 | 37.330 | 1.00 | 0.00 |
| ATOM | 828 | O | SER | S | 85 | 41.329 | 66.159 | 36.861 | 1.00 | 0.00 |
| ATOM | 829 | CB | SER | S | 85 | 39.373 | 68.579 | 36.848 | 1.00 | 0.00 |
| ATOM | 830 | OG | SER | S | 85 | 38.148 | 69.284 | 36.564 | 1.00 | 0.00 |
| ATOM | 831 | H | SER | S | 85 | 37.362 | 67.452 | 37.901 | 1.00 | 0.00 |
| ATOM | 832 | HG | SER | S | 85 | 37.788 | 68.927 | 35.743 | 1.00 | 0.00 |
| ATOM | 833 | N | GLY | S | 86 | 39.782 | 65.413 | 38.324 | 1.00 | 0.00 |
| ATOM | 834 | CA | GLY | S | 86 | 40.406 | 64.098 | 38.339 | 1.00 | 0.00 |
| ATOM | 835 | C | GLY | S | 86 | 39.816 | 63.238 | 37.231 | 1.00 | 0.00 |
| ATOM | 836 | O | GLY | S | 86 | 38.739 | 62.655 | 37.352 | 1.00 | 0.00 |
| ATOM | 837 | H | GLY | S | 86 | 38.992 | 65.624 | 38.892 | 1.00 | 0.00 |
| ATOM | 838 | N | LYS | S | 87 | 40.556 | 63.203 | 36.113 | 1.00 | 0.00 |
| ATOM | 839 | CA | LYS | S | 87 | 40.049 | 62.410 | 34.986 | 1.00 | 0.00 |
| ATOM | 840 | C | LYS | S | 87 | 39.928 | 60.918 | 35.246 | 1.00 | 0.00 |
| ATOM | 841 | O | LYS | S | 87 | 39.059 | 60.227 | 34.704 | 1.00 | 0.00 |
| ATOM | 842 | CB | LYS | S | 87 | 40.889 | 62.615 | 33.714 | 1.00 | 0.00 |
| ATOM | 843 | CG | LYS | S | 87 | 40.274 | 62.033 | 32.422 | 1.00 | 0.00 |
| ATOM | 844 | CD | LYS | S | 87 | 41.047 | 60.882 | 31.742 | 1.00 | 0.00 |
| ATOM | 845 | CE | LYS | S | 87 | 40.996 | 59.480 | 32.384 | 1.00 | 0.00 |
| ATOM | 846 | NZ | LYS | S | 87 | 39.639 | 58.919 | 32.358 | 1.00 | 0.00 |
| ATOM | 847 | H | LYS | S | 87 | 41.338 | 63.825 | 36.057 | 1.00 | 0.00 |
| ATOM | 848 | 1HZ | LYS | S | 87 | 39.548 | 58.068 | 32.952 | 1.00 | 0.00 |
| ATOM | 849 | 2HZ | LYS | S | 87 | 38.923 | 59.611 | 32.640 | 1.00 | 0.00 |
| ATOM | 850 | 3HZ | LYS | S | 87 | 39.406 | 58.670 | 31.387 | 1.00 | 0.00 |
| ATOM | 851 | N | VAL | S | 88 | 40.906 | 60.427 | 36.026 | 1.00 | 0.00 |
| ATOM | 852 | CA | VAL | S | 88 | 41.104 | 58.975 | 36.124 | 1.00 | 0.00 |
| ATOM | 853 | C | VAL | S | 88 | 40.245 | 58.362 | 37.217 | 1.00 | 0.00 |
| ATOM | 854 | O | VAL | S | 88 | 40.697 | 57.902 | 38.259 | 1.00 | 0.00 |
| ATOM | 855 | CB | VAL | S | 88 | 42.593 | 58.637 | 36.316 | 1.00 | 0.00 |
| ATOM | 856 | CG1 | VAL | S | 88 | 42.867 | 57.152 | 36.050 | 1.00 | 0.00 |
| ATOM | 857 | CG2 | VAL | S | 88 | 43.492 | 59.516 | 35.442 | 1.00 | 0.00 |
| ATOM | 858 | H | VAL | S | 88 | 41.394 | 61.070 | 36.623 | 1.00 | 0.00 |
| ATOM | 859 | N | PHE | S | 89 | 38.947 | 58.485 | 36.960 | 1.00 | 0.00 |
| ATOM | 860 | CA | PHE | S | 89 | 37.955 | 58.413 | 38.031 | 1.00 | 0.00 |
| ATOM | 861 | C | PHE | S | 89 | 36.565 | 58.084 | 37.501 | 1.00 | 0.00 |
| ATOM | 862 | O | PHE | S | 89 | 35.719 | 57.470 | 38.162 | 1.00 | 0.00 |
| ATOM | 863 | CB | PHE | S | 89 | 37.869 | 59.768 | 38.742 | 1.00 | 0.00 |
| ATOM | 864 | CG | PHE | S | 89 | 38.953 | 60.007 | 39.766 | 1.00 | 0.00 |
| ATOM | 865 | CD1 | PHE | S | 89 | 40.123 | 60.707 | 39.400 | 1.00 | 0.00 |
| ATOM | 866 | CD2 | PHE | S | 89 | 38.764 | 59.551 | 41.087 | 1.00 | 0.00 |
| ATOM | 867 | CE1 | PHE | S | 89 | 41.113 | 60.969 | 40.365 | 1.00 | 0.00 |
| ATOM | 868 | CE2 | PHE | S | 89 | 39.750 | 59.820 | 42.055 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 869 | CZ | PHE | S | 89 | 40.913 | 60.527 | 41.688 | 1.00 | 0.00 |
| ATOM | 870 | H | PHE | S | 89 | 38.696 | 58.685 | 36.014 | 1.00 | 0.00 |
| ATOM | 871 | N | ALA | S | 90 | 36.375 | 58.576 | 36.279 | 1.00 | 0.00 |
| ATOM | 872 | CA | ALA | S | 90 | 35.008 | 58.727 | 35.851 | 1.00 | 0.00 |
| ATOM | 873 | C | ALA | S | 90 | 34.774 | 58.235 | 34.451 | 1.00 | 0.00 |
| ATOM | 874 | O | ALA | S | 90 | 33.924 | 57.370 | 34.220 | 1.00 | 0.00 |
| ATOM | 875 | CB | ALA | S | 90 | 34.628 | 60.200 | 35.941 | 1.00 | 0.00 |
| ATOM | 876 | H | ALA | S | 90 | 37.131 | 58.885 | 35.712 | 1.00 | 0.00 |
| ATOM | 877 | N | SER | S | 91 | 35.498 | 58.903 | 33.529 | 1.00 | 0.00 |
| ATOM | 878 | CA | SER | S | 91 | 35.294 | 58.720 | 32.093 | 1.00 | 0.00 |
| ATOM | 879 | C | SER | S | 91 | 36.303 | 59.548 | 31.294 | 1.00 | 0.00 |
| ATOM | 880 | O | SER | S | 91 | 37.175 | 60.215 | 31.856 | 1.00 | 0.00 |
| ATOM | 881 | CB | SER | S | 91 | 33.843 | 59.074 | 31.732 | 1.00 | 0.00 |
| ATOM | 882 | OG | SER | S | 91 | 33.374 | 58.246 | 30.663 | 1.00 | 0.00 |
| ATOM | 883 | H | SER | S | 91 | 36.156 | 59.596 | 33.820 | 1.00 | 0.00 |
| ATOM | 884 | HG | SER | S | 91 | 32.463 | 58.051 | 30.895 | 1.00 | 0.00 |
| ATOM | 885 | N | THR | S | 92 | 36.171 | 59.491 | 29.954 | 1.00 | 0.00 |
| ATOM | 886 | CA | THR | S | 92 | 37.181 | 60.090 | 29.064 | 1.00 | 0.00 |
| ATOM | 887 | C | THR | S | 92 | 36.570 | 60.520 | 27.716 | 1.00 | 0.00 |
| ATOM | 888 | O | THR | S | 92 | 35.387 | 60.297 | 27.452 | 1.00 | 0.00 |
| ATOM | 889 | CB | THR | S | 92 | 38.333 | 59.071 | 28.866 | 1.00 | 0.00 |
| ATOM | 890 | OG1 | THR | S | 92 | 38.515 | 58.246 | 30.036 | 1.00 | 0.00 |
| ATOM | 891 | CG2 | THR | S | 92 | 39.672 | 59.717 | 28.509 | 1.00 | 0.00 |
| ATOM | 892 | H | THR | S | 92 | 35.403 | 58.982 | 29.560 | 1.00 | 0.00 |
| ATOM | 893 | HG1 | THR | S | 92 | 37.743 | 57.674 | 30.050 | 1.00 | 0.00 |
| ATOM | 894 | N | GLY | S | 93 | 37.394 | 61.118 | 26.838 | 1.00 | 0.00 |
| ATOM | 895 | CA | GLY | S | 93 | 37.063 | 61.027 | 25.415 | 1.00 | 0.00 |
| ATOM | 896 | C | GLY | S | 93 | 37.102 | 59.588 | 24.943 | 1.00 | 0.00 |
| ATOM | 897 | O | GLY | S | 93 | 37.438 | 58.686 | 25.716 | 1.00 | 0.00 |
| ATOM | 898 | H | GLY | S | 93 | 38.315 | 61.335 | 27.147 | 1.00 | 0.00 |
| ATOM | 899 | N | TYR | S | 94 | 36.706 | 59.408 | 23.679 | 1.00 | 0.00 |
| ATOM | 900 | CA | TYR | S | 94 | 36.531 | 58.024 | 23.231 | 1.00 | 0.00 |
| ATOM | 901 | C | TYR | S | 94 | 37.493 | 57.677 | 22.112 | 1.00 | 0.00 |
| ATOM | 902 | O | TYR | S | 94 | 38.180 | 58.554 | 21.586 | 1.00 | 0.00 |
| ATOM | 903 | CB | TYR | S | 94 | 35.133 | 57.753 | 22.660 | 1.00 | 0.00 |
| ATOM | 904 | CG | TYR | S | 94 | 33.943 | 58.480 | 23.254 | 1.00 | 0.00 |
| ATOM | 905 | CD1 | TYR | S | 94 | 33.886 | 58.972 | 24.578 | 1.00 | 0.00 |
| ATOM | 906 | CD2 | TYR | S | 94 | 32.851 | 58.608 | 22.384 | 1.00 | 0.00 |
| ATOM | 907 | CE1 | TYR | S | 94 | 32.685 | 59.536 | 25.049 | 1.00 | 0.00 |
| ATOM | 908 | CE2 | TYR | S | 94 | 31.660 | 59.178 | 22.839 | 1.00 | 0.00 |
| ATOM | 909 | CZ | TYR | S | 94 | 31.578 | 59.593 | 24.176 | 1.00 | 0.00 |
| ATOM | 910 | OH | TYR | S | 94 | 30.350 | 60.036 | 24.621 | 1.00 | 0.00 |
| ATOM | 911 | H | TYR | S | 94 | 36.484 | 60.220 | 23.139 | 1.00 | 0.00 |
| ATOM | 912 | HH | TYR | S | 94 | 29.962 | 60.600 | 23.928 | 1.00 | 0.00 |
| ATOM | 913 | N | GLY | S | 95 | 37.465 | 56.402 | 21.672 | 1.00 | 0.00 |
| ATOM | 914 | CA | GLY | S | 95 | 37.841 | 56.165 | 20.271 | 1.00 | 0.00 |
| ATOM | 915 | C | GLY | S | 95 | 38.438 | 54.798 | 19.991 | 1.00 | 0.00 |
| ATOM | 916 | O | GLY | S | 95 | 38.497 | 53.966 | 20.906 | 1.00 | 0.00 |
| ATOM | 917 | H | GLY | S | 95 | 37.010 | 55.705 | 22.228 | 1.00 | 0.00 |
| ATOM | 918 | N | ILE | S | 96 | 38.887 | 54.651 | 18.724 | 1.00 | 0.00 |
| ATOM | 919 | CA | ILE | S | 96 | 39.271 | 53.342 | 18.188 | 1.00 | 0.00 |
| ATOM | 920 | C | ILE | S | 96 | 40.610 | 52.785 | 18.620 | 1.00 | 0.00 |
| ATOM | 921 | O | ILE | S | 96 | 40.868 | 51.578 | 18.502 | 1.00 | 0.00 |
| ATOM | 922 | CB | ILE | S | 96 | 39.132 | 53.285 | 16.651 | 1.00 | 0.00 |
| ATOM | 923 | CG1 | ILE | S | 96 | 40.215 | 54.068 | 15.901 | 1.00 | 0.00 |
| ATOM | 924 | CG2 | ILE | S | 96 | 37.739 | 53.765 | 16.230 | 1.00 | 0.00 |
| ATOM | 925 | CD1 | ILE | S | 96 | 41.445 | 53.238 | 15.519 | 1.00 | 0.00 |
| ATOM | 926 | H | ILE | S | 96 | 38.882 | 55.462 | 18.143 | 1.00 | 0.00 |
| ATOM | 927 | N | ALA | S | 97 | 41.460 | 53.710 | 19.107 | 1.00 | 0.00 |
| ATOM | 928 | CA | ALA | S | 97 | 42.791 | 53.251 | 19.499 | 1.00 | 0.00 |
| ATOM | 929 | C | ALA | S | 97 | 42.748 | 52.110 | 20.492 | 1.00 | 0.00 |
| ATOM | 930 | O | ALA | S | 97 | 41.833 | 51.938 | 21.297 | 1.00 | 0.00 |
| ATOM | 931 | CB | ALA | S | 97 | 43.670 | 54.390 | 20.006 | 1.00 | 0.00 |
| ATOM | 932 | H | ALA | S | 97 | 41.172 | 54.656 | 19.227 | 1.00 | 0.00 |
| ATOM | 933 | N | ILE | S | 98 | 43.711 | 51.210 | 20.276 | 1.00 | 0.00 |
| ATOM | 934 | CA | ILE | S | 98 | 43.448 | 49.845 | 20.725 | 1.00 | 0.00 |
| ATOM | 935 | C | ILE | S | 98 | 44.463 | 49.310 | 21.688 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 936 | O | ILE | S | 98 | 45.672 | 49.486 | 21.519 | 1.00 | 0.00 |
| ATOM | 937 | CB | ILE | S | 98 | 43.323 | 48.844 | 19.568 | 1.00 | 0.00 |
| ATOM | 938 | CG1 | ILE | S | 98 | 44.277 | 49.065 | 18.385 | 1.00 | 0.00 |
| ATOM | 939 | CG2 | ILE | S | 98 | 41.870 | 48.755 | 19.122 | 1.00 | 0.00 |
| ATOM | 940 | CD1 | ILE | S | 98 | 43.820 | 50.105 | 17.352 | 1.00 | 0.00 |
| ATOM | 941 | H | ILE | S | 98 | 44.496 | 51.476 | 19.719 | 1.00 | 0.00 |
| ATOM | 942 | N | GLN | S | 99 | 43.900 | 48.594 | 22.670 | 1.00 | 0.00 |
| ATOM | 943 | CA | GLN | S | 99 | 44.708 | 47.780 | 23.577 | 1.00 | 0.00 |
| ATOM | 944 | C | GLN | S | 99 | 45.915 | 48.502 | 24.175 | 1.00 | 0.00 |
| ATOM | 945 | O | GLN | S | 99 | 45.815 | 49.664 | 24.556 | 1.00 | 0.00 |
| ATOM | 946 | CB | GLN | S | 99 | 45.073 | 46.479 | 22.868 | 1.00 | 0.00 |
| ATOM | 947 | CG | GLN | S | 99 | 43.911 | 45.741 | 22.210 | 1.00 | 0.00 |
| ATOM | 948 | CD | GLN | S | 99 | 44.491 | 44.457 | 21.690 | 1.00 | 0.00 |
| ATOM | 949 | OE1 | GLN | S | 99 | 44.690 | 44.258 | 20.493 | 1.00 | 0.00 |
| ATOM | 950 | NE2 | GLN | S | 99 | 44.860 | 43.629 | 22.670 | 1.00 | 0.00 |
| ATOM | 951 | H | GLN | S | 99 | 42.900 | 48.570 | 22.664 | 1.00 | 0.00 |
| ATOM | 952 | 1HE2 | GLN | S | 99 | 45.332 | 42.757 | 22.571 | 1.00 | 0.00 |
| ATOM | 953 | 2HE2 | GLN | S | 99 | 44.692 | 43.952 | 23.603 | 1.00 | 0.00 |
| ATOM | 954 | N | LYS | S | 100 | 47.060 | 47.811 | 24.190 | 1.00 | 0.00 |
| ATOM | 955 | CA | LYS | S | 100 | 48.340 | 48.507 | 24.267 | 1.00 | 0.00 |
| ATOM | 956 | C | LYS | S | 100 | 49.201 | 48.097 | 23.068 | 1.00 | 0.00 |
| ATOM | 957 | O | LYS | S | 100 | 50.416 | 47.959 | 23.128 | 1.00 | 0.00 |
| ATOM | 958 | CB | LYS | S | 100 | 48.992 | 48.198 | 25.621 | 1.00 | 0.00 |
| ATOM | 959 | CG | LYS | S | 100 | 49.863 | 49.311 | 26.224 | 1.00 | 0.00 |
| ATOM | 960 | CD | LYS | S | 100 | 49.107 | 50.555 | 26.720 | 1.00 | 0.00 |
| ATOM | 961 | CE | LYS | S | 100 | 48.076 | 50.270 | 27.823 | 1.00 | 0.00 |
| ATOM | 962 | NZ | LYS | S | 100 | 47.492 | 51.508 | 28.355 | 1.00 | 0.00 |
| ATOM | 963 | H | LYS | S | 100 | 47.076 | 46.819 | 24.084 | 1.00 | 0.00 |
| ATOM | 964 | 1HZ | LYS | S | 100 | 46.789 | 51.304 | 29.089 | 1.00 | 0.00 |
| ATOM | 965 | 2HZ | LYS | S | 100 | 47.066 | 52.118 | 27.637 | 1.00 | 0.00 |
| ATOM | 966 | 3HZ | LYS | S | 100 | 48.200 | 52.042 | 28.897 | 1.00 | 0.00 |
| ATOM | 967 | N | ASP | S | 101 | 48.457 | 47.835 | 21.963 | 1.00 | 0.00 |
| ATOM | 968 | CA | ASP | S | 101 | 48.959 | 46.952 | 20.896 | 1.00 | 0.00 |
| ATOM | 969 | C | ASP | S | 101 | 50.017 | 47.491 | 19.941 | 1.00 | 0.00 |
| ATOM | 970 | O | ASP | S | 101 | 50.317 | 48.679 | 19.904 | 1.00 | 0.00 |
| ATOM | 971 | CB | ASP | S | 101 | 47.776 | 46.387 | 20.100 | 1.00 | 0.00 |
| ATOM | 972 | CG | ASP | S | 101 | 47.999 | 44.911 | 19.831 | 1.00 | 0.00 |
| ATOM | 973 | OD1 | ASP | S | 101 | 48.389 | 44.540 | 18.729 | 1.00 | 0.00 |
| ATOM | 974 | OD2 | ASP | S | 101 | 47.782 | 44.111 | 20.731 | 1.00 | 0.00 |
| ATOM | 975 | H | ASP | S | 101 | 47.491 | 48.095 | 21.953 | 1.00 | 0.00 |
| ATOM | 976 | N | SER | S | 102 | 50.571 | 46.560 | 19.147 | 1.00 | 0.00 |
| ATOM | 977 | CA | SER | S | 102 | 51.574 | 46.936 | 18.144 | 1.00 | 0.00 |
| ATOM | 978 | C | SER | S | 102 | 51.303 | 46.460 | 16.714 | 1.00 | 0.00 |
| ATOM | 979 | O | SER | S | 102 | 52.129 | 46.591 | 15.800 | 1.00 | 0.00 |
| ATOM | 980 | CB | SER | S | 102 | 52.964 | 46.486 | 18.598 | 1.00 | 0.00 |
| ATOM | 981 | OG | SER | S | 102 | 53.362 | 47.153 | 19.813 | 1.00 | 0.00 |
| ATOM | 982 | H | SER | S | 102 | 50.284 | 45.604 | 19.249 | 1.00 | 0.00 |
| ATOM | 983 | HG | SER | S | 102 | 52.603 | 47.676 | 20.084 | 1.00 | 0.00 |
| ATOM | 984 | N | GLY | S | 103 | 50.093 | 45.892 | 16.551 | 1.00 | 0.00 |
| ATOM | 985 | CA | GLY | S | 103 | 49.648 | 45.634 | 15.184 | 1.00 | 0.00 |
| ATOM | 986 | C | GLY | S | 103 | 49.051 | 46.858 | 14.517 | 1.00 | 0.00 |
| ATOM | 987 | O | GLY | S | 103 | 49.553 | 47.356 | 13.496 | 1.00 | 0.00 |
| ATOM | 988 | H | GLY | S | 103 | 49.531 | 45.620 | 17.332 | 1.00 | 0.00 |
| ATOM | 989 | N | TRP | S | 104 | 47.952 | 47.280 | 15.167 | 1.00 | 0.00 |
| ATOM | 990 | CA | TRP | S | 104 | 47.125 | 48.393 | 14.687 | 1.00 | 0.00 |
| ATOM | 991 | C | TRP | S | 104 | 47.502 | 49.709 | 15.369 | 1.00 | 0.00 |
| ATOM | 992 | O | TRP | S | 104 | 47.716 | 50.766 | 14.776 | 1.00 | 0.00 |
| ATOM | 993 | CB | TRP | S | 104 | 45.666 | 47.989 | 14.957 | 1.00 | 0.00 |
| ATOM | 994 | CG | TRP | S | 104 | 44.623 | 48.376 | 13.919 | 1.00 | 0.00 |
| ATOM | 995 | CD1 | TRP | S | 104 | 43.246 | 48.498 | 14.181 | 1.00 | 0.00 |
| ATOM | 996 | CD2 | TRP | S | 104 | 44.744 | 48.613 | 12.494 | 1.00 | 0.00 |
| ATOM | 997 | NE1 | TRP | S | 104 | 42.533 | 48.780 | 13.057 | 1.00 | 0.00 |
| ATOM | 998 | CE2 | TRP | S | 104 | 43.419 | 48.859 | 11.991 | 1.00 | 0.00 |
| ATOM | 999 | CE3 | TRP | S | 104 | 45.835 | 48.620 | 11.598 | 1.00 | 0.00 |
| ATOM | 1000 | CZ2 | TRP | S | 104 | 43.218 | 49.108 | 10.616 | 1.00 | 0.00 |
| ATOM | 1001 | CZ3 | TRP | S | 104 | 45.621 | 48.864 | 10.226 | 1.00 | 0.00 |
| ATOM | 1002 | CH2 | TRP | S | 104 | 44.320 | 49.109 | 9.737 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1003 | H | TRP | S | 104 | 47.668 | 46.707 | 15.934 | 1.00 | 0.00 |
| ATOM | 1004 | HE1 | TRP | S | 104 | 41.554 | 48.899 | 12.981 | 1.00 | 0.00 |
| ATOM | 1005 | N | LYS | S | 105 | 47.638 | 49.597 | 16.717 | 1.00 | 0.00 |
| ATOM | 1006 | CA | LYS | S | 105 | 47.976 | 50.818 | 17.459 | 1.00 | 0.00 |
| ATOM | 1007 | C | LYS | S | 105 | 49.259 | 51.497 | 16.993 | 1.00 | 0.00 |
| ATOM | 1008 | O | LYS | S | 105 | 49.341 | 52.716 | 16.896 | 1.00 | 0.00 |
| ATOM | 1009 | CB | LYS | S | 105 | 47.971 | 50.631 | 18.990 | 1.00 | 0.00 |
| ATOM | 1010 | CG | LYS | S | 105 | 47.254 | 51.783 | 19.720 | 1.00 | 0.00 |
| ATOM | 1011 | CD | LYS | S | 105 | 47.955 | 52.379 | 20.956 | 1.00 | 0.00 |
| ATOM | 1012 | CE | LYS | S | 105 | 48.075 | 51.540 | 22.243 | 1.00 | 0.00 |
| ATOM | 1013 | NZ | LYS | S | 105 | 46.807 | 51.410 | 22.972 | 1.00 | 0.00 |
| ATOM | 1014 | H | LYS | S | 105 | 47.383 | 48.741 | 17.166 | 1.00 | 0.00 |
| ATOM | 1015 | 1HZ | LYS | S | 105 | 46.200 | 52.250 | 22.946 | 1.00 | 0.00 |
| ATOM | 1016 | 2HZ | LYS | S | 105 | 46.985 | 51.264 | 23.985 | 1.00 | 0.00 |
| ATOM | 1017 | 3HZ | LYS | S | 105 | 46.245 | 50.584 | 22.703 | 1.00 | 0.00 |
| ATOM | 1018 | N | ARG | S | 106 | 50.261 | 50.671 | 16.648 | 1.00 | 0.00 |
| ATOM | 1019 | CA | ARG | S | 106 | 51.404 | 51.262 | 15.943 | 1.00 | 0.00 |
| ATOM | 1020 | C | ARG | S | 106 | 51.192 | 51.458 | 14.434 | 1.00 | 0.00 |
| ATOM | 1021 | O | ARG | S | 106 | 51.752 | 50.778 | 13.569 | 1.00 | 0.00 |
| ATOM | 1022 | CB | ARG | S | 106 | 52.674 | 50.472 | 16.261 | 1.00 | 0.00 |
| ATOM | 1023 | CG | ARG | S | 106 | 53.006 | 50.343 | 17.758 | 1.00 | 0.00 |
| ATOM | 1024 | CD | ARG | S | 106 | 53.783 | 51.492 | 18.421 | 1.00 | 0.00 |
| ATOM | 1025 | NE | ARG | S | 106 | 52.971 | 52.649 | 18.806 | 1.00 | 0.00 |
| ATOM | 1026 | CZ | ARG | S | 106 | 53.125 | 53.225 | 20.029 | 1.00 | 0.00 |
| ATOM | 1027 | NH1 | ARG | S | 106 | 52.463 | 54.337 | 20.317 | 1.00 | 0.00 |
| ATOM | 1028 | NH2 | ARG | S | 106 | 53.932 | 52.698 | 20.951 | 1.00 | 0.00 |
| ATOM | 1029 | H | ARG | S | 106 | 50.121 | 49.684 | 16.692 | 1.00 | 0.00 |
| ATOM | 1030 | HE | ARG | S | 106 | 52.358 | 53.098 | 18.144 | 1.00 | 0.00 |
| ATOM | 1031 | 1HH1 | ARG | S | 106 | 52.502 | 54.793 | 21.200 | 1.00 | 0.00 |
| ATOM | 1032 | 2HH1 | ARG | S | 106 | 51.906 | 54.799 | 19.603 | 1.00 | 0.00 |
| ATOM | 1033 | 1HH2 | ARG | S | 106 | 54.069 | 53.164 | 21.825 | 1.00 | 0.00 |
| ATOM | 1034 | 2HH2 | ARG | S | 106 | 54.414 | 51.840 | 20.792 | 1.00 | 0.00 |
| ATOM | 1035 | N | GLN | S | 107 | 50.344 | 52.470 | 14.204 | 1.00 | 0.00 |
| ATOM | 1036 | CA | GLN | S | 107 | 49.863 | 53.021 | 12.932 | 1.00 | 0.00 |
| ATOM | 1037 | C | GLN | S | 107 | 48.911 | 54.152 | 13.298 | 1.00 | 0.00 |
| ATOM | 1038 | O | GLN | S | 107 | 48.974 | 55.295 | 12.833 | 1.00 | 0.00 |
| ATOM | 1039 | CB | GLN | S | 107 | 49.111 | 51.994 | 12.067 | 1.00 | 0.00 |
| ATOM | 1040 | CG | GLN | S | 107 | 48.685 | 52.536 | 10.692 | 1.00 | 0.00 |
| ATOM | 1041 | CD | GLN | S | 107 | 47.396 | 51.865 | 10.257 | 1.00 | 0.00 |
| ATOM | 1042 | OE1 | GLN | S | 107 | 46.416 | 51.845 | 10.989 | 1.00 | 0.00 |
| ATOM | 1043 | NE2 | GLN | S | 107 | 47.434 | 51.294 | 9.054 | 1.00 | 0.00 |
| ATOM | 1044 | H | GLN | S | 107 | 50.093 | 52.968 | 15.035 | 1.00 | 0.00 |
| ATOM | 1045 | 1HE2 | GLN | S | 107 | 46.668 | 50.743 | 8.730 | 1.00 | 0.00 |
| ATOM | 1046 | 2HE2 | GLN | S | 107 | 48.231 | 51.392 | 8.461 | 1.00 | 0.00 |
| ATOM | 1047 | N | VAL | S | 108 | 48.034 | 53.764 | 14.238 | 1.00 | 0.00 |
| ATOM | 1048 | CA | VAL | S | 108 | 47.092 | 54.702 | 14.843 | 1.00 | 0.00 |
| ATOM | 1049 | C | VAL | S | 108 | 47.704 | 55.952 | 15.472 | 1.00 | 0.00 |
| ATOM | 1050 | O | VAL | S | 108 | 47.102 | 57.025 | 15.408 | 1.00 | 0.00 |
| ATOM | 1051 | CB | VAL | S | 108 | 46.132 | 53.964 | 15.798 | 1.00 | 0.00 |
| ATOM | 1052 | CG1 | VAL | S | 108 | 45.127 | 54.884 | 16.498 | 1.00 | 0.00 |
| ATOM | 1053 | CG2 | VAL | S | 108 | 45.374 | 52.882 | 15.025 | 1.00 | 0.00 |
| ATOM | 1054 | H | VAL | S | 108 | 47.968 | 52.778 | 14.401 | 1.00 | 0.00 |
| ATOM | 1055 | N | ASP | S | 109 | 48.925 | 55.834 | 16.025 | 1.00 | 0.00 |
| ATOM | 1056 | CA | ASP | S | 109 | 49.694 | 57.029 | 16.426 | 1.00 | 0.00 |
| ATOM | 1057 | C | ASP | S | 109 | 49.580 | 58.213 | 15.473 | 1.00 | 0.00 |
| ATOM | 1058 | O | ASP | S | 109 | 49.420 | 59.378 | 15.821 | 1.00 | 0.00 |
| ATOM | 1059 | CB | ASP | S | 109 | 51.183 | 56.698 | 16.538 | 1.00 | 0.00 |
| ATOM | 1060 | CG | ASP | S | 109 | 51.480 | 55.902 | 17.785 | 1.00 | 0.00 |
| ATOM | 1061 | OD1 | ASP | S | 109 | 51.953 | 56.480 | 18.755 | 1.00 | 0.00 |
| ATOM | 1062 | OD2 | ASP | S | 109 | 51.261 | 54.695 | 17.799 | 1.00 | 0.00 |
| ATOM | 1063 | H | ASP | S | 109 | 49.293 | 54.915 | 16.177 | 1.00 | 0.00 |
| ATOM | 1064 | N | LEU | S | 110 | 49.678 | 57.839 | 14.188 | 1.00 | 0.00 |
| ATOM | 1065 | CA | LEU | S | 110 | 49.443 | 58.873 | 13.185 | 1.00 | 0.00 |
| ATOM | 1066 | C | LEU | S | 110 | 47.995 | 59.353 | 13.165 | 1.00 | 0.00 |
| ATOM | 1067 | O | LEU | S | 110 | 47.692 | 60.520 | 13.406 | 1.00 | 0.00 |
| ATOM | 1068 | CB | LEU | S | 110 | 49.922 | 58.371 | 11.819 | 1.00 | 0.00 |
| ATOM | 1069 | CG | LEU | S | 110 | 50.131 | 59.472 | 10.779 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1070 | CD1 | LEU | S | 110 | 51.175 | 60.499 | 11.224 | 1.00 | 0.00 |
| ATOM | 1071 | CD2 | LEU | S | 110 | 50.446 | 58.892 | 9.400 | 1.00 | 0.00 |
| ATOM | 1072 | H | LEU | S | 110 | 49.695 | 56.858 | 13.980 | 1.00 | 0.00 |
| ATOM | 1073 | N | ALA | S | 111 | 47.106 | 58.376 | 12.892 | 1.00 | 0.00 |
| ATOM | 1074 | CA | ALA | S | 111 | 45.657 | 58.607 | 12.780 | 1.00 | 0.00 |
| ATOM | 1075 | C | ALA | S | 111 | 44.990 | 59.653 | 13.669 | 1.00 | 0.00 |
| ATOM | 1076 | O | ALA | S | 111 | 44.345 | 60.568 | 13.171 | 1.00 | 0.00 |
| ATOM | 1077 | CB | ALA | S | 111 | 44.892 | 57.290 | 12.920 | 1.00 | 0.00 |
| ATOM | 1078 | H | ALA | S | 111 | 47.472 | 57.479 | 12.653 | 1.00 | 0.00 |
| ATOM | 1079 | N | ILE | S | 112 | 45.164 | 59.520 | 14.994 | 1.00 | 0.00 |
| ATOM | 1080 | CA | ILE | S | 112 | 44.490 | 60.472 | 15.892 | 1.00 | 0.00 |
| ATOM | 1081 | C | ILE | S | 112 | 44.690 | 61.959 | 15.548 | 1.00 | 0.00 |
| ATOM | 1082 | O | ILE | S | 112 | 43.781 | 62.773 | 15.394 | 1.00 | 0.00 |
| ATOM | 1083 | CB | ILE | S | 112 | 44.836 | 60.110 | 17.355 | 1.00 | 0.00 |
| ATOM | 1084 | CG1 | ILE | S | 112 | 44.206 | 61.051 | 18.385 | 1.00 | 0.00 |
| ATOM | 1085 | CG2 | ILE | S | 112 | 46.352 | 59.980 | 17.582 | 1.00 | 0.00 |
| ATOM | 1086 | CD1 | ILE | S | 112 | 44.343 | 60.520 | 19.814 | 1.00 | 0.00 |
| ATOM | 1087 | H | ILE | S | 112 | 45.642 | 58.699 | 15.305 | 1.00 | 0.00 |
| ATOM | 1088 | N | LEU | S | 113 | 45.981 | 62.273 | 15.352 | 1.00 | 0.00 |
| ATOM | 1089 | CA | LEU | S | 113 | 46.331 | 63.634 | 14.942 | 1.00 | 0.00 |
| ATOM | 1090 | C | LEU | S | 113 | 46.027 | 63.887 | 13.473 | 1.00 | 0.00 |
| ATOM | 1091 | O | LEU | S | 113 | 45.802 | 64.997 | 13.007 | 1.00 | 0.00 |
| ATOM | 1092 | CB | LEU | S | 113 | 47.806 | 63.891 | 15.264 | 1.00 | 0.00 |
| ATOM | 1093 | CG | LEU | S | 113 | 48.242 | 65.355 | 15.141 | 1.00 | 0.00 |
| ATOM | 1094 | CD1 | LEU | S | 113 | 47.464 | 66.271 | 16.089 | 1.00 | 0.00 |
| ATOM | 1095 | CD2 | LEU | S | 113 | 49.754 | 65.507 | 15.310 | 1.00 | 0.00 |
| ATOM | 1096 | H | LEU | S | 113 | 46.647 | 61.526 | 15.356 | 1.00 | 0.00 |
| ATOM | 1097 | N | GLN | S | 114 | 46.017 | 62.764 | 12.740 | 1.00 | 0.00 |
| ATOM | 1098 | CA | GLN | S | 114 | 45.555 | 62.852 | 11.360 | 1.00 | 0.00 |
| ATOM | 1099 | C | GLN | S | 114 | 44.055 | 62.981 | 11.184 | 1.00 | 0.00 |
| ATOM | 1100 | O | GLN | S | 114 | 43.565 | 62.949 | 10.060 | 1.00 | 0.00 |
| ATOM | 1101 | CB | GLN | S | 114 | 46.038 | 61.656 | 10.538 | 1.00 | 0.00 |
| ATOM | 1102 | CG | GLN | S | 114 | 47.470 | 61.772 | 10.022 | 1.00 | 0.00 |
| ATOM | 1103 | CD | GLN | S | 114 | 47.546 | 62.702 | 8.826 | 1.00 | 0.00 |
| ATOM | 1104 | OE1 | GLN | S | 114 | 46.591 | 63.340 | 8.393 | 1.00 | 0.00 |
| ATOM | 1105 | NE2 | GLN | S | 114 | 48.760 | 62.773 | 8.269 | 1.00 | 0.00 |
| ATOM | 1106 | H | GLN | S | 114 | 46.132 | 61.855 | 13.138 | 1.00 | 0.00 |
| ATOM | 1107 | 1HE2 | GLN | S | 114 | 48.948 | 63.398 | 7.516 | 1.00 | 0.00 |
| ATOM | 1108 | 2HE2 | GLN | S | 114 | 49.467 | 62.176 | 8.649 | 1.00 | 0.00 |
| ATOM | 1109 | N | LEU | S | 115 | 43.294 | 63.159 | 12.284 | 1.00 | 0.00 |
| ATOM | 1110 | CA | LEU | S | 115 | 41.865 | 63.449 | 12.104 | 1.00 | 0.00 |
| ATOM | 1111 | C | LEU | S | 115 | 41.659 | 64.697 | 11.254 | 1.00 | 0.00 |
| ATOM | 1112 | O | LEU | S | 115 | 41.399 | 64.607 | 10.051 | 1.00 | 0.00 |
| ATOM | 1113 | CB | LEU | S | 115 | 41.151 | 63.503 | 13.460 | 1.00 | 0.00 |
| ATOM | 1114 | CG | LEU | S | 115 | 40.301 | 62.263 | 13.774 | 1.00 | 0.00 |
| ATOM | 1115 | CD1 | LEU | S | 115 | 41.090 | 60.953 | 13.724 | 1.00 | 0.00 |
| ATOM | 1116 | CD2 | LEU | S | 115 | 39.568 | 62.418 | 15.106 | 1.00 | 0.00 |
| ATOM | 1117 | H | LEU | S | 115 | 43.699 | 62.996 | 13.184 | 1.00 | 0.00 |
| ATOM | 1118 | N | PHE | S | 116 | 41.949 | 65.850 | 11.887 | 1.00 | 0.00 |
| ATOM | 1119 | CA | PHE | S | 116 | 42.256 | 67.030 | 11.072 | 1.00 | 0.00 |
| ATOM | 1120 | C | PHE | S | 116 | 43.417 | 66.739 | 10.138 | 1.00 | 0.00 |
| ATOM | 1121 | O | PHE | S | 116 | 44.210 | 65.835 | 10.389 | 1.00 | 0.00 |
| ATOM | 1122 | CB | PHE | S | 116 | 42.612 | 68.234 | 11.950 | 1.00 | 0.00 |
| ATOM | 1123 | CG | PHE | S | 116 | 41.426 | 68.713 | 12.755 | 1.00 | 0.00 |
| ATOM | 1124 | CD1 | PHE | S | 116 | 41.358 | 68.411 | 14.133 | 1.00 | 0.00 |
| ATOM | 1125 | CD2 | PHE | S | 116 | 40.412 | 69.465 | 12.121 | 1.00 | 0.00 |
| ATOM | 1126 | CE1 | PHE | S | 116 | 40.261 | 68.868 | 14.889 | 1.00 | 0.00 |
| ATOM | 1127 | CE2 | PHE | S | 116 | 39.314 | 69.923 | 12.876 | 1.00 | 0.00 |
| ATOM | 1128 | CZ | PHE | S | 116 | 39.250 | 69.620 | 14.253 | 1.00 | 0.00 |
| ATOM | 1129 | H | PHE | S | 116 | 41.978 | 65.878 | 12.883 | 1.00 | 0.00 |
| ATOM | 1130 | N | GLY | S | 117 | 43.469 | 67.518 | 9.055 | 1.00 | 0.00 |
| ATOM | 1131 | CA | GLY | S | 117 | 44.564 | 67.256 | 8.133 | 1.00 | 0.00 |
| ATOM | 1132 | C | GLY | S | 117 | 44.148 | 67.061 | 6.689 | 1.00 | 0.00 |
| ATOM | 1133 | O | GLY | S | 117 | 44.975 | 67.169 | 5.783 | 1.00 | 0.00 |
| ATOM | 1134 | H | GLY | S | 117 | 42.793 | 68.234 | 8.900 | 1.00 | 0.00 |
| ATOM | 1135 | N | ASP | S | 118 | 42.849 | 66.775 | 6.503 | 1.00 | 0.00 |
| ATOM | 1136 | CA | ASP | S | 118 | 42.378 | 66.502 | 5.142 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1137 | C | ASP | S | 118 | 41.245 | 67.378 | 4.630 | 1.00 | 0.00 |
| ATOM | 1138 | O | ASP | S | 118 | 41.159 | 67.699 | 3.446 | 1.00 | 0.00 |
| ATOM | 1139 | CB | ASP | S | 118 | 42.054 | 65.007 | 4.959 | 1.00 | 0.00 |
| ATOM | 1140 | CG | ASP | S | 118 | 40.852 | 64.504 | 5.760 | 1.00 | 0.00 |
| ATOM | 1141 | OD1 | ASP | S | 118 | 40.196 | 63.578 | 5.311 | 1.00 | 0.00 |
| ATOM | 1142 | OD2 | ASP | S | 118 | 40.571 | 64.975 | 6.857 | 1.00 | 0.00 |
| ATOM | 1143 | H | ASP | S | 118 | 42.250 | 66.696 | 7.296 | 1.00 | 0.00 |
| ATOM | 1144 | N | GLY | S | 119 | 40.392 | 67.760 | 5.588 | 1.00 | 0.00 |
| ATOM | 1145 | CA | GLY | S | 119 | 39.146 | 68.433 | 5.235 | 1.00 | 0.00 |
| ATOM | 1146 | C | GLY | S | 119 | 37.994 | 67.567 | 5.699 | 1.00 | 0.00 |
| ATOM | 1147 | O | GLY | S | 119 | 38.109 | 66.346 | 5.730 | 1.00 | 0.00 |
| ATOM | 1148 | H | GLY | S | 119 | 40.511 | 67.416 | 6.516 | 1.00 | 0.00 |
| ATOM | 1149 | N | GLU | S | 120 | 36.897 | 68.227 | 6.096 | 1.00 | 0.00 |
| ATOM | 1150 | CA | GLU | S | 120 | 35.812 | 67.552 | 6.828 | 1.00 | 0.00 |
| ATOM | 1151 | C | GLU | S | 120 | 36.212 | 66.816 | 8.101 | 1.00 | 0.00 |
| ATOM | 1152 | O | GLU | S | 120 | 36.528 | 65.617 | 8.145 | 1.00 | 0.00 |
| ATOM | 1153 | CB | GLU | S | 120 | 34.898 | 66.689 | 5.932 | 1.00 | 0.00 |
| ATOM | 1154 | CG | GLU | S | 120 | 33.740 | 66.075 | 6.740 | 1.00 | 0.00 |
| ATOM | 1155 | CD | GLU | S | 120 | 32.630 | 65.549 | 5.858 | 1.00 | 0.00 |
| ATOM | 1156 | OE1 | GLU | S | 120 | 32.671 | 64.406 | 5.411 | 1.00 | 0.00 |
| ATOM | 1157 | OE2 | GLU | S | 120 | 31.667 | 66.272 | 5.647 | 1.00 | 0.00 |
| ATOM | 1158 | H | GLU | S | 120 | 36.924 | 69.220 | 6.012 | 1.00 | 0.00 |
| ATOM | 1159 | N | MET | S | 121 | 36.152 | 67.604 | 9.176 | 1.00 | 0.00 |
| ATOM | 1160 | CA | MET | S | 121 | 35.877 | 66.980 | 10.465 | 1.00 | 0.00 |
| ATOM | 1161 | C | MET | S | 121 | 34.520 | 67.469 | 10.914 | 1.00 | 0.00 |
| ATOM | 1162 | O | MET | S | 121 | 33.773 | 68.004 | 10.099 | 1.00 | 0.00 |
| ATOM | 1163 | CB | MET | S | 121 | 36.966 | 67.275 | 11.490 | 1.00 | 0.00 |
| ATOM | 1164 | CG | MET | S | 121 | 38.083 | 66.240 | 11.401 | 1.00 | 0.00 |
| ATOM | 1165 | SD | MET | S | 121 | 39.087 | 66.227 | 12.889 | 1.00 | 0.00 |
| ATOM | 1166 | CE | MET | S | 121 | 37.793 | 65.770 | 14.053 | 1.00 | 0.00 |
| ATOM | 1167 | H | MET | S | 121 | 35.972 | 68.583 | 9.065 | 1.00 | 0.00 |
| ATOM | 1168 | N | GLU | S | 122 | 34.200 | 67.255 | 12.198 | 1.00 | 0.00 |
| ATOM | 1169 | CA | GLU | S | 122 | 33.031 | 67.868 | 12.838 | 1.00 | 0.00 |
| ATOM | 1170 | C | GLU | S | 122 | 31.650 | 67.366 | 12.433 | 1.00 | 0.00 |
| ATOM | 1171 | O | GLU | S | 122 | 30.779 | 67.227 | 13.277 | 1.00 | 0.00 |
| ATOM | 1172 | CB | GLU | S | 122 | 33.147 | 69.399 | 12.868 | 1.00 | 0.00 |
| ATOM | 1173 | CG | GLU | S | 122 | 34.276 | 69.818 | 13.820 | 1.00 | 0.00 |
| ATOM | 1174 | CD | GLU | S | 122 | 34.660 | 71.277 | 13.646 | 1.00 | 0.00 |
| ATOM | 1175 | OE1 | GLU | S | 122 | 35.846 | 71.548 | 13.484 | 1.00 | 0.00 |
| ATOM | 1176 | OE2 | GLU | S | 122 | 33.791 | 72.147 | 13.668 | 1.00 | 0.00 |
| ATOM | 1177 | H | GLU | S | 122 | 34.826 | 66.716 | 12.764 | 1.00 | 0.00 |
| ATOM | 1178 | N | GLU | S | 123 | 31.448 | 66.997 | 11.145 | 1.00 | 0.00 |
| ATOM | 1179 | CA | GLU | S | 123 | 30.161 | 66.346 | 10.811 | 1.00 | 0.00 |
| ATOM | 1180 | C | GLU | S | 123 | 29.875 | 65.117 | 11.656 | 1.00 | 0.00 |
| ATOM | 1181 | O | GLU | S | 123 | 28.766 | 64.847 | 12.113 | 1.00 | 0.00 |
| ATOM | 1182 | CB | GLU | S | 123 | 30.046 | 65.907 | 9.333 | 1.00 | 0.00 |
| ATOM | 1183 | CG | GLU | S | 123 | 28.596 | 65.538 | 8.927 | 1.00 | 0.00 |
| ATOM | 1184 | CD | GLU | S | 123 | 28.426 | 64.162 | 8.262 | 1.00 | 0.00 |
| ATOM | 1185 | OE1 | GLU | S | 123 | 27.388 | 63.913 | 7.647 | 1.00 | 0.00 |
| ATOM | 1186 | OE2 | GLU | S | 123 | 29.312 | 63.311 | 8.312 | 1.00 | 0.00 |
| ATOM | 1187 | H | GLU | S | 123 | 32.130 | 67.214 | 10.449 | 1.00 | 0.00 |
| ATOM | 1188 | N | LEU | S | 124 | 30.965 | 64.353 | 11.804 | 1.00 | 0.00 |
| ATOM | 1189 | CA | LEU | S | 124 | 30.872 | 63.071 | 12.497 | 1.00 | 0.00 |
| ATOM | 1190 | C | LEU | S | 124 | 30.817 | 63.249 | 14.004 | 1.00 | 0.00 |
| ATOM | 1191 | O | LEU | S | 124 | 30.121 | 62.565 | 14.747 | 1.00 | 0.00 |
| ATOM | 1192 | CB | LEU | S | 124 | 32.068 | 62.183 | 12.137 | 1.00 | 0.00 |
| ATOM | 1193 | CG | LEU | S | 124 | 32.648 | 62.336 | 10.722 | 1.00 | 0.00 |
| ATOM | 1194 | CD1 | LEU | S | 124 | 34.074 | 61.795 | 10.650 | 1.00 | 0.00 |
| ATOM | 1195 | CD2 | LEU | S | 124 | 31.766 | 61.732 | 9.631 | 1.00 | 0.00 |
| ATOM | 1196 | H | LEU | S | 124 | 31.849 | 64.676 | 11.473 | 1.00 | 0.00 |
| ATOM | 1197 | N | GLU | S | 125 | 31.605 | 64.233 | 14.449 | 1.00 | 0.00 |
| ATOM | 1198 | CA | GLU | S | 125 | 31.795 | 64.397 | 15.884 | 1.00 | 0.00 |
| ATOM | 1199 | C | GLU | S | 125 | 30.717 | 65.224 | 16.592 | 1.00 | 0.00 |
| ATOM | 1200 | O | GLU | S | 125 | 30.331 | 64.973 | 17.730 | 1.00 | 0.00 |
| ATOM | 1201 | CB | GLU | S | 125 | 33.221 | 64.920 | 16.120 | 1.00 | 0.00 |
| ATOM | 1202 | CG | GLU | S | 125 | 34.376 | 63.963 | 15.728 | 1.00 | 0.00 |
| ATOM | 1203 | CD | GLU | S | 125 | 34.526 | 63.709 | 14.226 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1204 | OE1 | GLU | S | 125 | 34.298 | 64.601 | 13.422 | 1.00 | 0.00 |
| ATOM | 1205 | OE2 | GLU | S | 125 | 34.873 | 62.605 | 13.828 | 1.00 | 0.00 |
| ATOM | 1206 | H | GLU | S | 125 | 32.164 | 64.731 | 13.783 | 1.00 | 0.00 |
| ATOM | 1207 | N | ALA | S | 126 | 30.229 | 66.235 | 15.872 | 1.00 | 0.00 |
| ATOM | 1208 | CA | ALA | S | 126 | 29.213 | 67.084 | 16.485 | 1.00 | 0.00 |
| ATOM | 1209 | C | ALA | S | 126 | 27.818 | 66.486 | 16.529 | 1.00 | 0.00 |
| ATOM | 1210 | O | ALA | S | 126 | 27.037 | 66.751 | 17.444 | 1.00 | 0.00 |
| ATOM | 1211 | CB | ALA | S | 126 | 29.144 | 68.446 | 15.792 | 1.00 | 0.00 |
| ATOM | 1212 | H | ALA | S | 126 | 30.546 | 66.399 | 14.942 | 1.00 | 0.00 |
| ATOM | 1213 | N | LEU | S | 127 | 27.516 | 65.655 | 15.521 | 1.00 | 0.00 |
| ATOM | 1214 | CA | LEU | S | 127 | 26.113 | 65.238 | 15.416 | 1.00 | 0.00 |
| ATOM | 1215 | C | LEU | S | 127 | 25.641 | 64.098 | 16.309 | 1.00 | 0.00 |
| ATOM | 1216 | O | LEU | S | 127 | 24.553 | 63.538 | 16.155 | 1.00 | 0.00 |
| ATOM | 1217 | CB | LEU | S | 127 | 25.703 | 64.985 | 13.962 | 1.00 | 0.00 |
| ATOM | 1218 | CG | LEU | S | 127 | 25.273 | 66.252 | 13.209 | 1.00 | 0.00 |
| ATOM | 1219 | CD1 | LEU | S | 127 | 26.445 | 67.142 | 12.785 | 1.00 | 0.00 |
| ATOM | 1220 | CD2 | LEU | S | 127 | 24.366 | 65.916 | 12.025 | 1.00 | 0.00 |
| ATOM | 1221 | H | LEU | S | 127 | 28.245 | 65.345 | 14.913 | 1.00 | 0.00 |
| ATOM | 1222 | N | TRP | S | 128 | 26.499 | 63.743 | 17.279 | 1.00 | 0.00 |
| ATOM | 1223 | CA | TRP | S | 128 | 26.044 | 62.945 | 18.425 | 1.00 | 0.00 |
| ATOM | 1224 | C | TRP | S | 128 | 25.475 | 63.754 | 19.594 | 1.00 | 0.00 |
| ATOM | 1225 | O | TRP | S | 128 | 24.333 | 63.612 | 20.034 | 1.00 | 0.00 |
| ATOM | 1226 | CB | TRP | S | 128 | 27.189 | 62.050 | 18.920 | 1.00 | 0.00 |
| ATOM | 1227 | CG | TRP | S | 128 | 26.680 | 60.737 | 19.476 | 1.00 | 0.00 |
| ATOM | 1228 | CD1 | TRP | S | 128 | 25.812 | 59.856 | 18.824 | 1.00 | 0.00 |
| ATOM | 1229 | CD2 | TRP | S | 128 | 26.992 | 60.088 | 20.732 | 1.00 | 0.00 |
| ATOM | 1230 | NE1 | TRP | S | 128 | 25.576 | 58.743 | 19.558 | 1.00 | 0.00 |
| ATOM | 1231 | CE2 | TRP | S | 128 | 26.280 | 58.838 | 20.750 | 1.00 | 0.00 |
| ATOM | 1232 | CE3 | TRP | S | 128 | 27.802 | 60.439 | 21.831 | 1.00 | 0.00 |
| ATOM | 1233 | CZ2 | TRP | S | 128 | 26.389 | 57.974 | 21.860 | 1.00 | 0.00 |
| ATOM | 1234 | CZ3 | TRP | S | 128 | 27.903 | 59.566 | 22.935 | 1.00 | 0.00 |
| ATOM | 1235 | CH2 | TRP | S | 128 | 27.201 | 58.342 | 22.952 | 1.00 | 0.00 |
| ATOM | 1236 | H | TRP | S | 128 | 27.441 | 64.075 | 17.221 | 1.00 | 0.00 |
| ATOM | 1237 | HE1 | TRP | S | 128 | 25.019 | 58.001 | 19.222 | 1.00 | 0.00 |
| ATOM | 1238 | N | LEU | S | 129 | 26.339 | 64.625 | 20.146 | 1.00 | 0.00 |
| ATOM | 1239 | CA | LEU | S | 129 | 25.974 | 65.195 | 21.449 | 1.00 | 0.00 |
| ATOM | 1240 | C | LEU | S | 129 | 26.073 | 66.696 | 21.620 | 1.00 | 0.00 |
| ATOM | 1241 | O | LEU | S | 129 | 25.309 | 67.308 | 22.363 | 1.00 | 0.00 |
| ATOM | 1242 | CB | LEU | S | 129 | 26.772 | 64.524 | 22.563 | 1.00 | 0.00 |
| ATOM | 1243 | CG | LEU | S | 129 | 25.939 | 63.688 | 23.529 | 1.00 | 0.00 |
| ATOM | 1244 | CD1 | LEU | S | 129 | 26.842 | 62.790 | 24.370 | 1.00 | 0.00 |
| ATOM | 1245 | CD2 | LEU | S | 129 | 25.015 | 64.547 | 24.394 | 1.00 | 0.00 |
| ATOM | 1246 | H | LEU | S | 129 | 27.243 | 64.726 | 19.723 | 1.00 | 0.00 |
| ATOM | 1247 | N | THR | S | 130 | 27.064 | 67.268 | 20.917 | 1.00 | 0.00 |
| ATOM | 1248 | CA | THR | S | 130 | 27.492 | 68.640 | 21.224 | 1.00 | 0.00 |
| ATOM | 1249 | C | THR | S | 130 | 28.073 | 68.787 | 22.649 | 1.00 | 0.00 |
| ATOM | 1250 | O | THR | S | 130 | 27.777 | 68.016 | 23.563 | 1.00 | 0.00 |
| ATOM | 1251 | CB | THR | S | 130 | 26.370 | 69.669 | 20.917 | 1.00 | 0.00 |
| ATOM | 1252 | OG1 | THR | S | 130 | 25.415 | 69.166 | 19.955 | 1.00 | 0.00 |
| ATOM | 1253 | CG2 | THR | S | 130 | 26.943 | 71.009 | 20.447 | 1.00 | 0.00 |
| ATOM | 1254 | H | THR | S | 130 | 27.560 | 66.698 | 20.262 | 1.00 | 0.00 |
| ATOM | 1255 | HG1 | THR | S | 130 | 25.891 | 68.572 | 19.374 | 1.00 | 0.00 |
| ATOM | 1256 | N | GLY | S | 131 | 28.970 | 69.768 | 22.821 | 1.00 | 0.00 |
| ATOM | 1257 | CA | GLY | S | 131 | 29.616 | 69.858 | 24.130 | 1.00 | 0.00 |
| ATOM | 1258 | C | GLY | S | 131 | 28.848 | 70.704 | 25.130 | 1.00 | 0.00 |
| ATOM | 1259 | O | GLY | S | 131 | 28.282 | 71.743 | 24.793 | 1.00 | 0.00 |
| ATOM | 1260 | H | GLY | S | 131 | 29.091 | 70.464 | 22.117 | 1.00 | 0.00 |
| ATOM | 1261 | N | ILE | S | 132 | 28.852 | 70.230 | 26.391 | 1.00 | 0.00 |
| ATOM | 1262 | CA | ILE | S | 132 | 28.154 | 70.973 | 27.454 | 1.00 | 0.00 |
| ATOM | 1263 | C | ILE | S | 132 | 28.816 | 70.916 | 28.842 | 1.00 | 0.00 |
| ATOM | 1264 | O | ILE | S | 132 | 28.885 | 71.906 | 29.591 | 1.00 | 0.00 |
| ATOM | 1265 | CB | ILE | S | 132 | 26.660 | 70.570 | 27.480 | 1.00 | 0.00 |
| ATOM | 1266 | CG1 | ILE | S | 132 | 25.848 | 71.320 | 28.544 | 1.00 | 0.00 |
| ATOM | 1267 | CG2 | ILE | S | 132 | 26.495 | 69.050 | 27.621 | 1.00 | 0.00 |
| ATOM | 1268 | CD1 | ILE | S | 132 | 24.357 | 70.973 | 28.534 | 1.00 | 0.00 |
| ATOM | 1269 | H | ILE | S | 132 | 29.188 | 69.303 | 26.552 | 1.00 | 0.00 |
| ATOM | 1270 | N | CYS | S | 133 | 29.328 | 69.701 | 29.123 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1271 | CA | CYS | S | 133 | 29.945 | 69.421 | 30.415 | 1.00 | 0.00 |
| ATOM | 1272 | C | CYS | S | 133 | 31.338 | 68.864 | 30.260 | 1.00 | 0.00 |
| ATOM | 1273 | O | CYS | S | 133 | 31.593 | 67.675 | 30.422 | 1.00 | 0.00 |
| ATOM | 1274 | CB | CYS | S | 133 | 29.086 | 68.449 | 31.227 | 1.00 | 0.00 |
| ATOM | 1275 | SG | CYS | S | 133 | 27.434 | 69.123 | 31.546 | 1.00 | 0.00 |
| ATOM | 1276 | H | CYS | S | 133 | 29.185 | 68.951 | 28.477 | 1.00 | 0.00 |
| ATOM | 1277 | N | HIS | S | 134 | 32.242 | 69.787 | 29.902 | 1.00 | 0.00 |
| ATOM | 1278 | CA | HIS | S | 134 | 33.629 | 69.332 | 29.867 | 1.00 | 0.00 |
| ATOM | 1279 | C | HIS | S | 134 | 34.344 | 69.363 | 31.218 | 1.00 | 0.00 |
| ATOM | 1280 | O | HIS | S | 134 | 33.816 | 69.844 | 32.226 | 1.00 | 0.00 |
| ATOM | 1281 | CB | HIS | S | 134 | 34.414 | 69.995 | 28.711 | 1.00 | 0.00 |
| ATOM | 1282 | CG | HIS | S | 134 | 34.398 | 69.097 | 27.481 | 1.00 | 0.00 |
| ATOM | 1283 | ND1 | HIS | S | 134 | 34.896 | 69.425 | 26.262 | 1.00 | 0.00 |
| ATOM | 1284 | CD2 | HIS | S | 134 | 33.881 | 67.800 | 27.396 | 1.00 | 0.00 |
| ATOM | 1285 | CE1 | HIS | S | 134 | 34.692 | 68.357 | 25.421 | 1.00 | 0.00 |
| ATOM | 1286 | NE2 | HIS | S | 134 | 34.069 | 67.356 | 26.129 | 1.00 | 0.00 |
| ATOM | 1287 | H | HIS | S | 134 | 31.958 | 70.744 | 29.945 | 1.00 | 0.00 |
| ATOM | 1288 | HD1 | HIS | S | 134 | 35.327 | 70.265 | 25.986 | 1.00 | 0.00 |
| ATOM | 1289 | N | ASN | S | 135 | 35.547 | 68.766 | 31.124 | 1.00 | 0.00 |
| ATOM | 1290 | CA | ASN | S | 135 | 36.329 | 68.169 | 32.209 | 1.00 | 0.00 |
| ATOM | 1291 | C | ASN | S | 135 | 36.632 | 69.030 | 33.435 | 1.00 | 0.00 |
| ATOM | 1292 | O | ASN | S | 135 | 35.783 | 69.152 | 34.318 | 1.00 | 0.00 |
| ATOM | 1293 | CB | ASN | S | 135 | 37.603 | 67.588 | 31.569 | 1.00 | 0.00 |
| ATOM | 1294 | CG | ASN | S | 135 | 38.202 | 66.477 | 32.407 | 1.00 | 0.00 |
| ATOM | 1295 | OD1 | ASN | S | 135 | 37.992 | 65.292 | 32.143 | 1.00 | 0.00 |
| ATOM | 1296 | ND2 | ASN | S | 135 | 38.960 | 66.901 | 33.414 | 1.00 | 0.00 |
| ATOM | 1297 | OXT | ASN | S | 135 | 37.738 | 69.557 | 33.521 | 1.00 | 0.00 |
| ATOM | 1298 | H | ASN | S | 135 | 35.805 | 68.433 | 30.220 | 1.00 | 0.00 |
| ATOM | 1299 | 1HD2 | ASN | S | 135 | 39.441 | 66.278 | 34.024 | 1.00 | 0.00 |
| ATOM | 1300 | 2HD2 | ASN | S | 135 | 39.039 | 67.886 | 33.547 | 1.00 | 0.00 |
| ATOM | 1301 | N | ASP | S | 1 | 49.744 | 46.793 | 10.820 | 1.00 | 0.00 |
| ATOM | 1302 | CA | ASP | S | 1 | 48.635 | 46.352 | 9.972 | 1.00 | 0.00 |
| ATOM | 1303 | C | ASP | S | 1 | 47.639 | 45.810 | 10.963 | 1.00 | 0.00 |
| ATOM | 1304 | O | ASP | S | 1 | 47.716 | 46.309 | 12.078 | 1.00 | 0.00 |
| ATOM | 1305 | CB | ASP | S | 1 | 49.130 | 45.338 | 8.934 | 1.00 | 0.00 |
| ATOM | 1306 | CG | ASP | S | 1 | 48.054 | 45.176 | 7.883 | 1.00 | 0.00 |
| ATOM | 1307 | OD1 | ASP | S | 1 | 47.751 | 44.061 | 7.486 | 1.00 | 0.00 |
| ATOM | 1308 | OD2 | ASP | S | 1 | 47.468 | 46.171 | 7.490 | 1.00 | 0.00 |
| ATOM | 1309 | 1H | ASP | S | 1 | 50.299 | 45.956 | 11.062 | 1.00 | 0.00 |
| ATOM | 1310 | 2H | ASP | S | 1 | 49.324 | 47.136 | 11.715 | 1.00 | 0.00 |
| ATOM | 1311 | 3H | ASP | S | 1 | 50.318 | 47.517 | 10.357 | 1.00 | 0.00 |
| ATOM | 1312 | N | ASP | S | 2 | 46.820 | 44.813 | 10.604 | 1.00 | 0.00 |
| ATOM | 1313 | CA | ASP | S | 2 | 46.003 | 44.088 | 11.579 | 1.00 | 0.00 |
| ATOM | 1314 | C | ASP | S | 2 | 45.233 | 43.023 | 10.818 | 1.00 | 0.00 |
| ATOM | 1315 | O | ASP | S | 2 | 45.835 | 42.266 | 10.061 | 1.00 | 0.00 |
| ATOM | 1316 | CB | ASP | S | 2 | 45.111 | 45.012 | 12.445 | 1.00 | 0.00 |
| ATOM | 1317 | CG | ASP | S | 2 | 44.375 | 44.208 | 13.501 | 1.00 | 0.00 |
| ATOM | 1318 | OD1 | ASP | S | 2 | 43.184 | 44.418 | 13.675 | 1.00 | 0.00 |
| ATOM | 1319 | OD2 | ASP | S | 2 | 44.963 | 43.313 | 14.093 | 1.00 | 0.00 |
| ATOM | 1320 | H | ASP | S | 2 | 46.873 | 44.427 | 9.681 | 1.00 | 0.00 |
| ATOM | 1321 | N | HIS | S | 3 | 43.896 | 43.011 | 10.969 | 1.00 | 0.00 |
| ATOM | 1322 | CA | HIS | S | 3 | 43.078 | 42.054 | 10.250 | 1.00 | 0.00 |
| ATOM | 1323 | C | HIS | S | 3 | 42.738 | 42.601 | 8.870 | 1.00 | 0.00 |
| ATOM | 1324 | O | HIS | S | 3 | 43.411 | 43.493 | 8.351 | 1.00 | 0.00 |
| ATOM | 1325 | CB | HIS | S | 3 | 41.855 | 41.741 | 11.126 | 1.00 | 0.00 |
| ATOM | 1326 | CG | HIS | S | 3 | 42.241 | 40.900 | 12.328 | 1.00 | 0.00 |
| ATOM | 1327 | ND1 | HIS | S | 3 | 42.867 | 41.359 | 13.433 | 1.00 | 0.00 |
| ATOM | 1328 | CD2 | HIS | S | 3 | 42.010 | 39.531 | 12.495 | 1.00 | 0.00 |
| ATOM | 1329 | CE1 | HIS | S | 3 | 43.028 | 40.299 | 14.281 | 1.00 | 0.00 |
| ATOM | 1330 | NE2 | HIS | S | 3 | 42.502 | 39.171 | 13.707 | 1.00 | 0.00 |
| ATOM | 1331 | H | HIS | S | 3 | 43.406 | 43.672 | 11.537 | 1.00 | 0.00 |
| ATOM | 1332 | HD1 | HIS | S | 3 | 43.121 | 42.291 | 13.638 | 1.00 | 0.00 |
| ATOM | 1333 | N | LEU | S | 4 | 41.679 | 42.012 | 8.277 | 1.00 | 0.00 |
| ATOM | 1334 | CA | LEU | S | 4 | 41.189 | 42.493 | 6.982 | 1.00 | 0.00 |
| ATOM | 1335 | C | LEU | S | 4 | 39.892 | 43.283 | 7.111 | 1.00 | 0.00 |
| ATOM | 1336 | O | LEU | S | 4 | 39.687 | 44.312 | 6.491 | 1.00 | 0.00 |
| ATOM | 1337 | CB | LEU | S | 4 | 41.046 | 41.328 | 6.002 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1338 | CG | LEU | S | 4 | 41.124 | 41.773 | 4.540 | 1.00 | 0.00 |
| ATOM | 1339 | CD1 | LEU | S | 4 | 42.483 | 42.396 | 4.211 | 1.00 | 0.00 |
| ATOM | 1340 | CD2 | LEU | S | 4 | 40.768 | 40.638 | 3.580 | 1.00 | 0.00 |
| ATOM | 1341 | H | LEU | S | 4 | 41.204 | 41.299 | 8.784 | 1.00 | 0.00 |
| ATOM | 1342 | N | SER | S | 5 | 39.061 | 42.785 | 8.040 | 1.00 | 0.00 |
| ATOM | 1343 | CA | SER | S | 5 | 38.086 | 43.683 | 8.651 | 1.00 | 0.00 |
| ATOM | 1344 | C | SER | S | 5 | 38.266 | 43.497 | 10.136 | 1.00 | 0.00 |
| ATOM | 1345 | O | SER | S | 5 | 38.631 | 42.415 | 10.594 | 1.00 | 0.00 |
| ATOM | 1346 | CB | SER | S | 5 | 36.652 | 43.347 | 8.221 | 1.00 | 0.00 |
| ATOM | 1347 | OG | SER | S | 5 | 35.729 | 44.343 | 8.693 | 1.00 | 0.00 |
| ATOM | 1348 | H | SER | S | 5 | 39.174 | 41.889 | 8.469 | 1.00 | 0.00 |
| ATOM | 1349 | HG | SER | S | 5 | 36.004 | 45.161 | 8.283 | 1.00 | 0.00 |
| ATOM | 1350 | N | ILE | S | 6 | 38.058 | 44.573 | 10.898 | 1.00 | 0.00 |
| ATOM | 1351 | CA | ILE | S | 6 | 38.289 | 44.386 | 12.321 | 1.00 | 0.00 |
| ATOM | 1352 | C | ILE | S | 6 | 37.041 | 44.553 | 13.154 | 1.00 | 0.00 |
| ATOM | 1353 | O | ILE | S | 6 | 36.376 | 45.590 | 13.243 | 1.00 | 0.00 |
| ATOM | 1354 | CB | ILE | S | 6 | 39.509 | 45.180 | 12.811 | 1.00 | 0.00 |
| ATOM | 1355 | CG1 | ILE | S | 6 | 39.847 | 44.799 | 14.251 | 1.00 | 0.00 |
| ATOM | 1356 | CG2 | ILE | S | 6 | 39.313 | 46.689 | 12.655 | 1.00 | 0.00 |
| ATOM | 1357 | CD1 | ILE | S | 6 | 40.062 | 43.292 | 14.426 | 1.00 | 0.00 |
| ATOM | 1358 | H | ILE | S | 6 | 37.693 | 45.412 | 10.489 | 1.00 | 0.00 |
| ATOM | 1359 | N | VAL | S | 7 | 36.685 | 43.390 | 13.721 | 1.00 | 0.00 |
| ATOM | 1360 | CA | VAL | S | 7 | 35.401 | 43.253 | 14.408 | 1.00 | 0.00 |
| ATOM | 1361 | C | VAL | S | 7 | 35.372 | 44.145 | 15.628 | 1.00 | 0.00 |
| ATOM | 1362 | O | VAL | S | 7 | 36.364 | 44.293 | 16.333 | 1.00 | 0.00 |
| ATOM | 1363 | CB | VAL | S | 7 | 35.157 | 41.784 | 14.799 | 1.00 | 0.00 |
| ATOM | 1364 | CG1 | VAL | S | 7 | 33.737 | 41.548 | 15.328 | 1.00 | 0.00 |
| ATOM | 1365 | CG2 | VAL | S | 7 | 35.477 | 40.833 | 13.642 | 1.00 | 0.00 |
| ATOM | 1366 | H | VAL | S | 7 | 37.390 | 42.675 | 13.700 | 1.00 | 0.00 |
| ATOM | 1367 | N | THR | S | 8 | 34.210 | 44.750 | 15.853 | 1.00 | 0.00 |
| ATOM | 1368 | CA | THR | S | 8 | 34.063 | 45.457 | 17.114 | 1.00 | 0.00 |
| ATOM | 1369 | C | THR | S | 8 | 32.693 | 45.271 | 17.737 | 1.00 | 0.00 |
| ATOM | 1370 | O | THR | S | 8 | 31.712 | 44.900 | 17.088 | 1.00 | 0.00 |
| ATOM | 1371 | CB | THR | S | 8 | 34.414 | 46.950 | 16.995 | 1.00 | 0.00 |
| ATOM | 1372 | OG1 | THR | S | 8 | 33.361 | 47.709 | 16.395 | 1.00 | 0.00 |
| ATOM | 1373 | CG2 | THR | S | 8 | 35.751 | 47.284 | 16.326 | 1.00 | 0.00 |
| ATOM | 1374 | H | THR | S | 8 | 33.436 | 44.599 | 15.240 | 1.00 | 0.00 |
| ATOM | 1375 | HG1 | THR | S | 8 | 33.504 | 47.639 | 15.443 | 1.00 | 0.00 |
| ATOM | 1376 | N | LEU | S | 9 | 32.635 | 45.560 | 19.042 | 1.00 | 0.00 |
| ATOM | 1377 | CA | LEU | S | 9 | 31.354 | 45.433 | 19.747 | 1.00 | 0.00 |
| ATOM | 1378 | C | LEU | S | 9 | 30.600 | 46.772 | 19.891 | 1.00 | 0.00 |
| ATOM | 1379 | O | LEU | S | 9 | 31.016 | 47.772 | 19.291 | 1.00 | 0.00 |
| ATOM | 1380 | CB | LEU | S | 9 | 31.585 | 44.720 | 21.094 | 1.00 | 0.00 |
| ATOM | 1381 | CG | LEU | S | 9 | 32.330 | 43.359 | 21.117 | 1.00 | 0.00 |
| ATOM | 1382 | CD1 | LEU | S | 9 | 32.185 | 42.486 | 19.865 | 1.00 | 0.00 |
| ATOM | 1383 | CD2 | LEU | S | 9 | 33.791 | 43.513 | 21.503 | 1.00 | 0.00 |
| ATOM | 1384 | H | LEU | S | 9 | 33.516 | 45.720 | 19.483 | 1.00 | 0.00 |
| ATOM | 1385 | N | GLU | S | 10 | 29.506 | 46.765 | 20.710 | 1.00 | 0.00 |
| ATOM | 1386 | CA | GLU | S | 10 | 28.582 | 47.901 | 20.917 | 1.00 | 0.00 |
| ATOM | 1387 | C | GLU | S | 10 | 27.429 | 47.495 | 21.850 | 1.00 | 0.00 |
| ATOM | 1388 | O | GLU | S | 10 | 27.438 | 46.364 | 22.346 | 1.00 | 0.00 |
| ATOM | 1389 | CB | GLU | S | 10 | 28.038 | 48.414 | 19.574 | 1.00 | 0.00 |
| ATOM | 1390 | CG | GLU | S | 10 | 26.969 | 47.549 | 18.895 | 1.00 | 0.00 |
| ATOM | 1391 | CD | GLU | S | 10 | 27.415 | 46.128 | 18.591 | 1.00 | 0.00 |
| ATOM | 1392 | OE1 | GLU | S | 10 | 27.741 | 45.846 | 17.443 | 1.00 | 0.00 |
| ATOM | 1393 | OE2 | GLU | S | 10 | 27.396 | 45.278 | 19.485 | 1.00 | 0.00 |
| ATOM | 1394 | H | GLU | S | 10 | 29.251 | 45.899 | 21.141 | 1.00 | 0.00 |
| ATOM | 1395 | N | GLU | S | 11 | 26.440 | 48.380 | 22.059 | 1.00 | 0.00 |
| ATOM | 1396 | CA | GLU | S | 11 | 25.271 | 47.952 | 22.834 | 1.00 | 0.00 |
| ATOM | 1397 | C | GLU | S | 11 | 23.963 | 48.403 | 22.209 | 1.00 | 0.00 |
| ATOM | 1398 | O | GLU | S | 11 | 23.938 | 49.142 | 21.222 | 1.00 | 0.00 |
| ATOM | 1399 | CB | GLU | S | 11 | 25.292 | 48.436 | 24.296 | 1.00 | 0.00 |
| ATOM | 1400 | CG | GLU | S | 11 | 26.631 | 48.458 | 25.043 | 1.00 | 0.00 |
| ATOM | 1401 | CD | GLU | S | 11 | 27.472 | 49.610 | 24.534 | 1.00 | 0.00 |
| ATOM | 1402 | OE1 | GLU | S | 11 | 26.974 | 50.731 | 24.513 | 1.00 | 0.00 |
| ATOM | 1403 | OE2 | GLU | S | 11 | 28.612 | 49.379 | 24.138 | 1.00 | 0.00 |
| ATOM | 1404 | H | GLU | S | 11 | 26.470 | 49.326 | 21.731 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1405 | N | ALA | S | 12 | 22.867 | 47.939 | 22.848 | 1.00 | 0.00 |
| ATOM | 1406 | CA | ALA | S | 12 | 21.536 | 48.436 | 22.493 | 1.00 | 0.00 |
| ATOM | 1407 | C | ALA | S | 12 | 20.925 | 49.575 | 23.329 | 1.00 | 0.00 |
| ATOM | 1408 | O | ALA | S | 12 | 20.366 | 50.503 | 22.745 | 1.00 | 0.00 |
| ATOM | 1409 | CB | ALA | S | 12 | 20.537 | 47.278 | 22.368 | 1.00 | 0.00 |
| ATOM | 1410 | H | ALA | S | 12 | 22.959 | 47.287 | 23.599 | 1.00 | 0.00 |
| ATOM | 1411 | N | PRO | S | 13 | 21.004 | 49.532 | 24.682 | 1.00 | 0.00 |
| ATOM | 1412 | CA | PRO | S | 13 | 20.454 | 50.678 | 25.413 | 1.00 | 0.00 |
| ATOM | 1413 | C | PRO | S | 13 | 21.219 | 51.987 | 25.232 | 1.00 | 0.00 |
| ATOM | 1414 | O | PRO | S | 13 | 22.229 | 52.215 | 25.905 | 1.00 | 0.00 |
| ATOM | 1415 | CB | PRO | S | 13 | 20.476 | 50.211 | 26.875 | 1.00 | 0.00 |
| ATOM | 1416 | CG | PRO | S | 13 | 20.632 | 48.692 | 26.834 | 1.00 | 0.00 |
| ATOM | 1417 | CD | PRO | S | 13 | 21.468 | 48.481 | 25.582 | 1.00 | 0.00 |
| ATOM | 1418 | N | PHE | S | 14 | 20.618 | 52.861 | 24.388 | 1.00 | 0.00 |
| ATOM | 1419 | CA | PHE | S | 14 | 20.975 | 54.269 | 24.116 | 1.00 | 0.00 |
| ATOM | 1420 | C | PHE | S | 14 | 21.665 | 54.447 | 22.786 | 1.00 | 0.00 |
| ATOM | 1421 | O | PHE | S | 14 | 21.248 | 55.205 | 21.918 | 1.00 | 0.00 |
| ATOM | 1422 | CB | PHE | S | 14 | 21.792 | 55.011 | 25.191 | 1.00 | 0.00 |
| ATOM | 1423 | CG | PHE | S | 14 | 20.913 | 55.522 | 26.309 | 1.00 | 0.00 |
| ATOM | 1424 | CD1 | PHE | S | 14 | 20.618 | 54.690 | 27.411 | 1.00 | 0.00 |
| ATOM | 1425 | CD2 | PHE | S | 14 | 20.416 | 56.842 | 26.237 | 1.00 | 0.00 |
| ATOM | 1426 | CE1 | PHE | S | 14 | 19.822 | 55.187 | 28.461 | 1.00 | 0.00 |
| ATOM | 1427 | CE2 | PHE | S | 14 | 19.620 | 57.342 | 27.286 | 1.00 | 0.00 |
| ATOM | 1428 | CZ | PHE | S | 14 | 19.335 | 56.510 | 28.390 | 1.00 | 0.00 |
| ATOM | 1429 | H | PHE | S | 14 | 19.915 | 52.441 | 23.809 | 1.00 | 0.00 |
| ATOM | 1430 | N | VAL | S | 15 | 22.749 | 53.669 | 22.607 | 1.00 | 0.00 |
| ATOM | 1431 | CA | VAL | S | 15 | 23.352 | 53.643 | 21.261 | 1.00 | 0.00 |
| ATOM | 1432 | C | VAL | S | 15 | 22.361 | 53.071 | 20.255 | 1.00 | 0.00 |
| ATOM | 1433 | O | VAL | S | 15 | 22.100 | 51.866 | 20.251 | 1.00 | 0.00 |
| ATOM | 1434 | CB | VAL | S | 15 | 24.671 | 52.851 | 21.260 | 1.00 | 0.00 |
| ATOM | 1435 | CG1 | VAL | S | 15 | 25.348 | 52.868 | 19.883 | 1.00 | 0.00 |
| ATOM | 1436 | CG2 | VAL | S | 15 | 25.619 | 53.364 | 22.348 | 1.00 | 0.00 |
| ATOM | 1437 | H | VAL | S | 15 | 22.981 | 52.979 | 23.296 | 1.00 | 0.00 |
| ATOM | 1438 | N | ILE | S | 16 | 21.751 | 54.033 | 19.549 | 1.00 | 0.00 |
| ATOM | 1439 | CA | ILE | S | 16 | 20.561 | 53.989 | 18.697 | 1.00 | 0.00 |
| ATOM | 1440 | C | ILE | S | 16 | 20.068 | 55.432 | 18.638 | 1.00 | 0.00 |
| ATOM | 1441 | O | ILE | S | 16 | 18.994 | 55.848 | 19.072 | 1.00 | 0.00 |
| ATOM | 1442 | CB | ILE | S | 16 | 19.483 | 52.965 | 19.151 | 1.00 | 0.00 |
| ATOM | 1443 | CG1 | ILE | S | 16 | 18.337 | 52.862 | 18.137 | 1.00 | 0.00 |
| ATOM | 1444 | CG2 | ILE | S | 16 | 18.941 | 53.214 | 20.571 | 1.00 | 0.00 |
| ATOM | 1445 | CD1 | ILE | S | 16 | 17.372 | 51.708 | 18.417 | 1.00 | 0.00 |
| ATOM | 1446 | H | ILE | S | 16 | 22.135 | 54.934 | 19.748 | 1.00 | 0.00 |
| ATOM | 1447 | N | VAL | S | 17 | 21.016 | 56.240 | 18.153 | 1.00 | 0.00 |
| ATOM | 1448 | CA | VAL | S | 17 | 20.794 | 57.681 | 18.084 | 1.00 | 0.00 |
| ATOM | 1449 | C | VAL | S | 17 | 20.423 | 58.090 | 16.673 | 1.00 | 0.00 |
| ATOM | 1450 | O | VAL | S | 17 | 19.427 | 58.761 | 16.428 | 1.00 | 0.00 |
| ATOM | 1451 | CB | VAL | S | 17 | 22.027 | 58.433 | 18.608 | 1.00 | 0.00 |
| ATOM | 1452 | CG1 | VAL | S | 17 | 21.865 | 59.956 | 18.543 | 1.00 | 0.00 |
| ATOM | 1453 | CG2 | VAL | S | 17 | 22.351 | 57.971 | 20.032 | 1.00 | 0.00 |
| ATOM | 1454 | H | VAL | S | 17 | 21.871 | 55.819 | 17.854 | 1.00 | 0.00 |
| ATOM | 1455 | N | GLU | S | 18 | 21.230 | 57.576 | 15.720 | 1.00 | 0.00 |
| ATOM | 1456 | CA | GLU | S | 18 | 20.732 | 57.639 | 14.341 | 1.00 | 0.00 |
| ATOM | 1457 | C | GLU | S | 18 | 19.763 | 56.499 | 14.090 | 1.00 | 0.00 |
| ATOM | 1458 | O | GLU | S | 18 | 20.124 | 55.452 | 13.542 | 1.00 | 0.00 |
| ATOM | 1459 | CB | GLU | S | 18 | 21.874 | 57.598 | 13.308 | 1.00 | 0.00 |
| ATOM | 1460 | CG | GLU | S | 18 | 21.440 | 57.875 | 11.851 | 1.00 | 0.00 |
| ATOM | 1461 | CD | GLU | S | 18 | 22.247 | 57.085 | 10.814 | 1.00 | 0.00 |
| ATOM | 1462 | OE1 | GLU | S | 18 | 22.923 | 56.121 | 11.143 | 1.00 | 0.00 |
| ATOM | 1463 | OE2 | GLU | S | 18 | 22.173 | 57.391 | 9.635 | 1.00 | 0.00 |
| ATOM | 1464 | H | GLU | S | 18 | 22.060 | 57.078 | 15.979 | 1.00 | 0.00 |
| ATOM | 1465 | N | SER | S | 19 | 18.522 | 56.730 | 14.535 | 1.00 | 0.00 |
| ATOM | 1466 | CA | SER | S | 19 | 17.440 | 55.771 | 14.297 | 1.00 | 0.00 |
| ATOM | 1467 | C | SER | S | 19 | 16.844 | 56.073 | 12.912 | 1.00 | 0.00 |
| ATOM | 1468 | O | SER | S | 19 | 17.666 | 56.457 | 12.079 | 1.00 | 0.00 |
| ATOM | 1469 | CB | SER | S | 19 | 16.587 | 55.788 | 15.574 | 1.00 | 0.00 |
| ATOM | 1470 | OG | SER | S | 19 | 17.496 | 55.713 | 16.677 | 1.00 | 0.00 |
| ATOM | 1471 | H | SER | S | 19 | 18.379 | 57.601 | 15.014 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1472 | HG | SER | S | 19 | 16.986 | 55.434 | 17.439 | 1.00 | 0.00 |
| ATOM | 1473 | N | VAL | S | 20 | 15.532 | 55.950 | 12.582 | 1.00 | 0.00 |
| ATOM | 1474 | CA | VAL | S | 20 | 14.345 | 55.479 | 13.312 | 1.00 | 0.00 |
| ATOM | 1475 | C | VAL | S | 20 | 13.948 | 54.131 | 12.728 | 1.00 | 0.00 |
| ATOM | 1476 | O | VAL | S | 20 | 14.323 | 53.850 | 11.589 | 1.00 | 0.00 |
| ATOM | 1477 | CB | VAL | S | 20 | 13.218 | 56.524 | 13.171 | 1.00 | 0.00 |
| ATOM | 1478 | CG1 | VAL | S | 20 | 11.993 | 56.225 | 14.043 | 1.00 | 0.00 |
| ATOM | 1479 | CG2 | VAL | S | 20 | 13.741 | 57.934 | 13.463 | 1.00 | 0.00 |
| ATOM | 1480 | H | VAL | S | 20 | 15.376 | 56.119 | 11.611 | 1.00 | 0.00 |
| ATOM | 1481 | N | ASP | S | 21 | 13.229 | 53.326 | 13.533 | 1.00 | 0.00 |
| ATOM | 1482 | CA | ASP | S | 21 | 13.250 | 51.883 | 13.272 | 1.00 | 0.00 |
| ATOM | 1483 | C | ASP | S | 21 | 11.928 | 51.144 | 12.945 | 1.00 | 0.00 |
| ATOM | 1484 | O | ASP | S | 21 | 11.537 | 50.185 | 13.612 | 1.00 | 0.00 |
| ATOM | 1485 | CB | ASP | S | 21 | 13.947 | 51.217 | 14.476 | 1.00 | 0.00 |
| ATOM | 1486 | CG | ASP | S | 21 | 15.458 | 51.452 | 14.556 | 1.00 | 0.00 |
| ATOM | 1487 | OD1 | ASP | S | 21 | 15.949 | 52.570 | 14.475 | 1.00 | 0.00 |
| ATOM | 1488 | OD2 | ASP | S | 21 | 16.186 | 50.490 | 14.715 | 1.00 | 0.00 |
| ATOM | 1489 | H | ASP | S | 21 | 12.879 | 53.640 | 14.411 | 1.00 | 0.00 |
| ATOM | 1490 | N | PRO | S | 22 | 11.196 | 51.569 | 11.872 | 1.00 | 0.00 |
| ATOM | 1491 | CA | PRO | S | 22 | 10.035 | 50.765 | 11.451 | 1.00 | 0.00 |
| ATOM | 1492 | C | PRO | S | 22 | 10.443 | 49.716 | 10.409 | 1.00 | 0.00 |
| ATOM | 1493 | O | PRO | S | 22 | 11.590 | 49.262 | 10.382 | 1.00 | 0.00 |
| ATOM | 1494 | CB | PRO | S | 22 | 9.117 | 51.872 | 10.924 | 1.00 | 0.00 |
| ATOM | 1495 | CG | PRO | S | 22 | 10.055 | 52.876 | 10.254 | 1.00 | 0.00 |
| ATOM | 1496 | CD | PRO | S | 22 | 11.348 | 52.772 | 11.057 | 1.00 | 0.00 |
| ATOM | 1497 | N | LEU | S | 23 | 9.510 | 49.373 | 9.510 | 1.00 | 0.00 |
| ATOM | 1498 | CA | LEU | S | 23 | 9.918 | 48.602 | 8.336 | 1.00 | 0.00 |
| ATOM | 1499 | C | LEU | S | 23 | 10.555 | 49.525 | 7.307 | 1.00 | 0.00 |
| ATOM | 1500 | O | LEU | S | 23 | 9.871 | 50.222 | 6.566 | 1.00 | 0.00 |
| ATOM | 1501 | CB | LEU | S | 23 | 8.678 | 47.889 | 7.778 | 1.00 | 0.00 |
| ATOM | 1502 | CG | LEU | S | 23 | 8.842 | 47.119 | 6.460 | 1.00 | 0.00 |
| ATOM | 1503 | CD1 | LEU | S | 23 | 9.863 | 45.988 | 6.551 | 1.00 | 0.00 |
| ATOM | 1504 | CD2 | LEU | S | 23 | 7.495 | 46.613 | 5.945 | 1.00 | 0.00 |
| ATOM | 1505 | H | LEU | S | 23 | 8.597 | 49.767 | 9.562 | 1.00 | 0.00 |
| ATOM | 1506 | N | SER | S | 24 | 11.892 | 49.552 | 7.297 | 1.00 | 0.00 |
| ATOM | 1507 | CA | SER | S | 24 | 12.517 | 50.557 | 6.440 | 1.00 | 0.00 |
| ATOM | 1508 | C | SER | S | 24 | 13.859 | 50.146 | 5.868 | 1.00 | 0.00 |
| ATOM | 1509 | O | SER | S | 24 | 14.932 | 50.552 | 6.308 | 1.00 | 0.00 |
| ATOM | 1510 | CB | SER | S | 24 | 12.573 | 51.927 | 7.139 | 1.00 | 0.00 |
| ATOM | 1511 | OG | SER | S | 24 | 11.232 | 52.412 | 7.359 | 1.00 | 0.00 |
| ATOM | 1512 | H | SER | S | 24 | 12.459 | 48.930 | 7.837 | 1.00 | 0.00 |
| ATOM | 1513 | HG | SER | S | 24 | 10.657 | 51.876 | 6.819 | 1.00 | 0.00 |
| ATOM | 1514 | N | GLY | S | 25 | 13.741 | 49.330 | 4.810 | 1.00 | 0.00 |
| ATOM | 1515 | CA | GLY | S | 25 | 14.960 | 48.996 | 4.075 | 1.00 | 0.00 |
| ATOM | 1516 | C | GLY | S | 25 | 15.455 | 50.082 | 3.134 | 1.00 | 0.00 |
| ATOM | 1517 | O | GLY | S | 25 | 15.577 | 49.905 | 1.919 | 1.00 | 0.00 |
| ATOM | 1518 | H | GLY | S | 25 | 12.855 | 48.939 | 4.570 | 1.00 | 0.00 |
| ATOM | 1519 | N | THR | S | 26 | 15.724 | 51.253 | 3.714 | 1.00 | 0.00 |
| ATOM | 1520 | CA | THR | S | 26 | 16.216 | 52.288 | 2.825 | 1.00 | 0.00 |
| ATOM | 1521 | C | THR | S | 26 | 17.737 | 52.362 | 2.715 | 1.00 | 0.00 |
| ATOM | 1522 | O | THR | S | 26 | 18.446 | 53.218 | 3.253 | 1.00 | 0.00 |
| ATOM | 1523 | CB | THR | S | 26 | 15.473 | 53.614 | 3.086 | 1.00 | 0.00 |
| ATOM | 1524 | OG1 | THR | S | 26 | 15.546 | 54.478 | 1.942 | 1.00 | 0.00 |
| ATOM | 1525 | CG2 | THR | S | 26 | 15.844 | 54.325 | 4.393 | 1.00 | 0.00 |
| ATOM | 1526 | H | THR | S | 26 | 15.696 | 51.364 | 4.707 | 1.00 | 0.00 |
| ATOM | 1527 | HG1 | THR | S | 26 | 16.332 | 55.006 | 2.043 | 1.00 | 0.00 |
| ATOM | 1528 | N | CYS | S | 27 | 18.196 | 51.397 | 1.895 | 1.00 | 0.00 |
| ATOM | 1529 | CA | CYS | S | 27 | 19.611 | 51.232 | 1.540 | 1.00 | 0.00 |
| ATOM | 1530 | C | CYS | S | 27 | 20.429 | 50.758 | 2.727 | 1.00 | 0.00 |
| ATOM | 1531 | O | CYS | S | 27 | 21.450 | 51.311 | 3.131 | 1.00 | 0.00 |
| ATOM | 1532 | CB | CYS | S | 27 | 20.198 | 52.496 | 0.885 | 1.00 | 0.00 |
| ATOM | 1533 | SG | CYS | S | 27 | 21.756 | 52.263 | -0.022 | 1.00 | 0.00 |
| ATOM | 1534 | H | CYS | S | 27 | 17.532 | 50.675 | 1.709 | 1.00 | 0.00 |
| ATOM | 1535 | N | MET | S | 28 | 19.884 | 49.699 | 3.339 | 1.00 | 0.00 |
| ATOM | 1536 | CA | MET | S | 28 | 20.582 | 49.186 | 4.511 | 1.00 | 0.00 |
| ATOM | 1537 | C | MET | S | 28 | 21.733 | 48.255 | 4.149 | 1.00 | 0.00 |
| ATOM | 1538 | O | MET | S | 28 | 21.757 | 47.739 | 3.028 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1539 | CB | MET | S | 28 | 19.560 | 48.599 | 5.485 | 1.00 | 0.00 |
| ATOM | 1540 | CG | MET | S | 28 | 18.646 | 49.715 | 5.993 | 1.00 | 0.00 |
| ATOM | 1541 | SD | MET | S | 28 | 17.842 | 49.313 | 7.543 | 1.00 | 0.00 |
| ATOM | 1542 | CE | MET | S | 28 | 17.069 | 47.771 | 7.031 | 1.00 | 0.00 |
| ATOM | 1543 | H | MET | S | 28 | 19.130 | 49.210 | 2.899 | 1.00 | 0.00 |
| ATOM | 1544 | N | ARG | S | 29 | 22.700 | 48.058 | 5.084 | 1.00 | 0.00 |
| ATOM | 1545 | CA | ARG | S | 29 | 22.798 | 48.584 | 6.459 | 1.00 | 0.00 |
| ATOM | 1546 | C | ARG | S | 29 | 22.903 | 50.092 | 6.680 | 1.00 | 0.00 |
| ATOM | 1547 | O | ARG | S | 29 | 22.746 | 50.584 | 7.794 | 1.00 | 0.00 |
| ATOM | 1548 | CB | ARG | S | 29 | 23.978 | 47.936 | 7.202 | 1.00 | 0.00 |
| ATOM | 1549 | CG | ARG | S | 29 | 23.848 | 46.440 | 7.493 | 1.00 | 0.00 |
| ATOM | 1550 | CD | ARG | S | 29 | 25.143 | 45.742 | 7.942 | 1.00 | 0.00 |
| ATOM | 1551 | NE | ARG | S | 29 | 25.662 | 46.198 | 9.236 | 1.00 | 0.00 |
| ATOM | 1552 | CZ | ARG | S | 29 | 26.510 | 45.417 | 9.947 | 1.00 | 0.00 |
| ATOM | 1553 | NH1 | ARG | S | 29 | 27.167 | 45.947 | 10.984 | 1.00 | 0.00 |
| ATOM | 1554 | NH2 | ARG | S | 29 | 26.690 | 44.142 | 9.591 | 1.00 | 0.00 |
| ATOM | 1555 | H | ARG | S | 29 | 23.326 | 47.344 | 4.786 | 1.00 | 0.00 |
| ATOM | 1556 | HE | ARG | S | 29 | 25.345 | 47.084 | 9.571 | 1.00 | 0.00 |
| ATOM | 1557 | 1HH1 | ARG | S | 29 | 27.745 | 45.381 | 11.588 | 1.00 | 0.00 |
| ATOM | 1558 | 2HH1 | ARG | S | 29 | 27.099 | 46.927 | 11.193 | 1.00 | 0.00 |
| ATOM | 1559 | 1HH2 | ARG | S | 29 | 27.343 | 43.536 | 10.045 | 1.00 | 0.00 |
| ATOM | 1560 | 2HH2 | ARG | S | 29 | 26.159 | 43.704 | 8.846 | 1.00 | 0.00 |
| ATOM | 1561 | N | ASN | S | 30 | 23.235 | 50.843 | 5.629 | 1.00 | 0.00 |
| ATOM | 1562 | CA | ASN | S | 30 | 23.732 | 52.150 | 6.059 | 1.00 | 0.00 |
| ATOM | 1563 | C | ASN | S | 30 | 22.968 | 53.391 | 5.636 | 1.00 | 0.00 |
| ATOM | 1564 | O | ASN | S | 30 | 23.517 | 54.466 | 5.384 | 1.00 | 0.00 |
| ATOM | 1565 | CB | ASN | S | 30 | 25.232 | 52.234 | 5.816 | 1.00 | 0.00 |
| ATOM | 1566 | CG | ASN | S | 30 | 25.865 | 53.256 | 6.735 | 1.00 | 0.00 |
| ATOM | 1567 | OD1 | ASN | S | 30 | 26.798 | 53.956 | 6.349 | 1.00 | 0.00 |
| ATOM | 1568 | ND2 | ASN | S | 30 | 25.405 | 53.292 | 7.994 | 1.00 | 0.00 |
| ATOM | 1569 | H | ASN | S | 30 | 23.097 | 50.593 | 4.670 | 1.00 | 0.00 |
| ATOM | 1570 | 1HD2 | ASN | S | 30 | 25.912 | 53.852 | 8.646 | 1.00 | 0.00 |
| ATOM | 1571 | 2HD2 | ASN | S | 30 | 24.586 | 52.807 | 8.290 | 1.00 | 0.00 |
| ATOM | 1572 | N | THR | S | 31 | 21.641 | 53.173 | 5.604 | 1.00 | 0.00 |
| ATOM | 1573 | CA | THR | S | 31 | 20.673 | 54.185 | 5.164 | 1.00 | 0.00 |
| ATOM | 1574 | C | THR | S | 31 | 21.062 | 54.957 | 3.899 | 1.00 | 0.00 |
| ATOM | 1575 | O | THR | S | 31 | 22.016 | 54.648 | 3.192 | 1.00 | 0.00 |
| ATOM | 1576 | CB | THR | S | 31 | 20.210 | 55.079 | 6.348 | 1.00 | 0.00 |
| ATOM | 1577 | OG1 | THR | S | 31 | 18.969 | 55.756 | 6.064 | 1.00 | 0.00 |
| ATOM | 1578 | CG2 | THR | S | 31 | 21.262 | 56.073 | 6.842 | 1.00 | 0.00 |
| ATOM | 1579 | H | THR | S | 31 | 21.365 | 52.243 | 5.833 | 1.00 | 0.00 |
| ATOM | 1580 | HG1 | THR | S | 31 | 18.851 | 56.381 | 6.783 | 1.00 | 0.00 |
| ATOM | 1581 | N | VAL | S | 32 | 20.269 | 56.000 | 3.600 | 1.00 | 0.00 |
| ATOM | 1582 | CA | VAL | S | 32 | 20.537 | 56.742 | 2.365 | 1.00 | 0.00 |
| ATOM | 1583 | C | VAL | S | 32 | 21.990 | 57.206 | 2.162 | 1.00 | 0.00 |
| ATOM | 1584 | O | VAL | S | 32 | 22.609 | 56.843 | 1.174 | 1.00 | 0.00 |
| ATOM | 1585 | CB | VAL | S | 32 | 19.496 | 57.860 | 2.142 | 1.00 | 0.00 |
| ATOM | 1586 | CG1 | VAL | S | 32 | 19.662 | 58.538 | 0.777 | 1.00 | 0.00 |
| ATOM | 1587 | CG2 | VAL | S | 32 | 18.073 | 57.322 | 2.322 | 1.00 | 0.00 |
| ATOM | 1588 | H | VAL | S | 32 | 19.546 | 56.232 | 4.253 | 1.00 | 0.00 |
| ATOM | 1589 | N | PRO | S | 33 | 22.575 | 58.000 | 3.103 | 1.00 | 0.00 |
| ATOM | 1590 | CA | PRO | S | 33 | 23.963 | 58.441 | 2.871 | 1.00 | 0.00 |
| ATOM | 1591 | C | PRO | S | 33 | 25.071 | 57.411 | 3.117 | 1.00 | 0.00 |
| ATOM | 1592 | O | PRO | S | 33 | 26.157 | 57.774 | 3.577 | 1.00 | 0.00 |
| ATOM | 1593 | CB | PRO | S | 33 | 24.119 | 59.639 | 3.820 | 1.00 | 0.00 |
| ATOM | 1594 | CG | PRO | S | 33 | 22.729 | 59.958 | 4.369 | 1.00 | 0.00 |
| ATOM | 1595 | CD | PRO | S | 33 | 22.027 | 58.612 | 4.308 | 1.00 | 0.00 |
| ATOM | 1596 | N | CYS | S | 34 | 24.775 | 56.130 | 2.817 | 1.00 | 0.00 |
| ATOM | 1597 | CA | CYS | S | 34 | 25.654 | 55.009 | 3.159 | 1.00 | 0.00 |
| ATOM | 1598 | C | CYS | S | 34 | 27.141 | 55.183 | 2.933 | 1.00 | 0.00 |
| ATOM | 1599 | O | CYS | S | 34 | 27.960 | 54.674 | 3.690 | 1.00 | 0.00 |
| ATOM | 1600 | CB | CYS | S | 34 | 25.173 | 53.729 | 2.465 | 1.00 | 0.00 |
| ATOM | 1601 | SG | CYS | S | 34 | 25.151 | 53.851 | 0.656 | 1.00 | 0.00 |
| ATOM | 1602 | H | CYS | S | 34 | 23.906 | 55.925 | 2.369 | 1.00 | 0.00 |
| ATOM | 1603 | N | GLN | S | 35 | 27.471 | 55.896 | 1.842 | 1.00 | 0.00 |
| ATOM | 1604 | CA | GLN | S | 35 | 28.906 | 56.052 | 1.639 | 1.00 | 0.00 |
| ATOM | 1605 | C | GLN | S | 35 | 29.504 | 57.413 | 1.923 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1606 | O | GLN | S | 35 | 30.721 | 57.578 | 1.880 | 1.00 | 0.00 |
| ATOM | 1607 | CB | GLN | S | 35 | 29.330 | 55.483 | 0.292 | 1.00 | 0.00 |
| ATOM | 1608 | CG | GLN | S | 35 | 29.199 | 53.960 | 0.334 | 1.00 | 0.00 |
| ATOM | 1609 | CD | GLN | S | 35 | 29.621 | 53.391 | -0.993 | 1.00 | 0.00 |
| ATOM | 1610 | OE1 | GLN | S | 35 | 30.793 | 53.284 | -1.328 | 1.00 | 0.00 |
| ATOM | 1611 | NE2 | GLN | S | 35 | 28.594 | 53.051 | -1.788 | 1.00 | 0.00 |
| ATOM | 1612 | H | GLN | S | 35 | 26.792 | 56.214 | 1.180 | 1.00 | 0.00 |
| ATOM | 1613 | 1HE2 | GLN | S | 35 | 28.832 | 52.764 | -2.719 | 1.00 | 0.00 |
| ATOM | 1614 | 2HE2 | GLN | S | 35 | 27.650 | 53.085 | -1.457 | 1.00 | 0.00 |
| ATOM | 1615 | N | LYS | S | 36 | 28.630 | 58.370 | 2.294 | 1.00 | 0.00 |
| ATOM | 1616 | CA | LYS | S | 36 | 29.197 | 59.577 | 2.911 | 1.00 | 0.00 |
| ATOM | 1617 | C | LYS | S | 36 | 29.636 | 59.280 | 4.339 | 1.00 | 0.00 |
| ATOM | 1618 | O | LYS | S | 36 | 30.815 | 59.217 | 4.684 | 1.00 | 0.00 |
| ATOM | 1619 | CB | LYS | S | 36 | 28.181 | 60.732 | 2.835 | 1.00 | 0.00 |
| ATOM | 1620 | CG | LYS | S | 36 | 28.693 | 62.175 | 3.016 | 1.00 | 0.00 |
| ATOM | 1621 | CD | LYS | S | 36 | 29.135 | 62.596 | 4.426 | 1.00 | 0.00 |
| ATOM | 1622 | CE | LYS | S | 36 | 29.413 | 64.103 | 4.515 | 1.00 | 0.00 |
| ATOM | 1623 | NZ | LYS | S | 36 | 29.846 | 64.465 | 5.865 | 1.00 | 0.00 |
| ATOM | 1624 | H | LYS | S | 36 | 27.668 | 58.125 | 2.386 | 1.00 | 0.00 |
| ATOM | 1625 | 1HZ | LYS | S | 36 | 30.882 | 64.508 | 5.946 | 1.00 | 0.00 |
| ATOM | 1626 | 2HZ | LYS | S | 36 | 29.533 | 65.416 | 6.124 | 1.00 | 0.00 |
| ATOM | 1627 | 3HZ | LYS | S | 36 | 29.477 | 63.849 | 6.609 | 1.00 | 0.00 |
| ATOM | 1628 | N | ARG | S | 37 | 28.614 | 59.019 | 5.171 | 1.00 | 0.00 |
| ATOM | 1629 | CA | ARG | S | 37 | 28.987 | 58.463 | 6.466 | 1.00 | 0.00 |
| ATOM | 1630 | C | ARG | S | 37 | 29.449 | 57.022 | 6.331 | 1.00 | 0.00 |
| ATOM | 1631 | O | ARG | S | 37 | 29.676 | 56.523 | 5.222 | 1.00 | 0.00 |
| ATOM | 1632 | CB | ARG | S | 37 | 27.845 | 58.667 | 7.465 | 1.00 | 0.00 |
| ATOM | 1633 | CG | ARG | S | 37 | 27.889 | 60.106 | 7.982 | 1.00 | 0.00 |
| ATOM | 1634 | CD | ARG | S | 37 | 26.840 | 60.455 | 9.037 | 1.00 | 0.00 |
| ATOM | 1635 | NE | ARG | S | 37 | 27.209 | 61.713 | 9.688 | 1.00 | 0.00 |
| ATOM | 1636 | CZ | ARG | S | 37 | 26.330 | 62.540 | 10.284 | 1.00 | 0.00 |
| ATOM | 1637 | NH1 | ARG | S | 37 | 26.772 | 63.573 | 10.991 | 1.00 | 0.00 |
| ATOM | 1638 | NH2 | ARG | S | 37 | 25.023 | 62.307 | 10.167 | 1.00 | 0.00 |
| ATOM | 1639 | H | ARG | S | 37 | 27.670 | 58.966 | 4.852 | 1.00 | 0.00 |
| ATOM | 1640 | HE | ARG | S | 37 | 28.177 | 62.000 | 9.621 | 1.00 | 0.00 |
| ATOM | 1641 | 1HH1 | ARG | S | 37 | 26.184 | 64.260 | 11.433 | 1.00 | 0.00 |
| ATOM | 1642 | 2HH1 | ARG | S | 37 | 27.763 | 63.741 | 11.118 | 1.00 | 0.00 |
| ATOM | 1643 | 1HH2 | ARG | S | 37 | 24.326 | 62.867 | 10.618 | 1.00 | 0.00 |
| ATOM | 1644 | 2HH2 | ARG | S | 37 | 24.697 | 61.543 | 9.607 | 1.00 | 0.00 |
| ATOM | 1645 | N | ILE | S | 38 | 29.637 | 56.397 | 7.490 | 1.00 | 0.00 |
| ATOM | 1646 | CA | ILE | S | 38 | 29.911 | 54.968 | 7.452 | 1.00 | 0.00 |
| ATOM | 1647 | C | ILE | S | 38 | 28.986 | 54.258 | 8.437 | 1.00 | 0.00 |
| ATOM | 1648 | O | ILE | S | 38 | 27.856 | 54.732 | 8.598 | 1.00 | 0.00 |
| ATOM | 1649 | CB | ILE | S | 38 | 31.433 | 54.727 | 7.537 | 1.00 | 0.00 |
| ATOM | 1650 | CG1 | ILE | S | 38 | 31.883 | 53.317 | 7.126 | 1.00 | 0.00 |
| ATOM | 1651 | CG2 | ILE | S | 38 | 31.976 | 55.173 | 8.892 | 1.00 | 0.00 |
| ATOM | 1652 | CD1 | ILE | S | 38 | 33.398 | 53.143 | 7.020 | 1.00 | 0.00 |
| ATOM | 1653 | H | ILE | S | 38 | 29.561 | 56.889 | 8.361 | 1.00 | 0.00 |
| ATOM | 1654 | N | ILE | S | 39 | 29.394 | 53.122 | 9.023 | 1.00 | 0.00 |
| ATOM | 1655 | CA | ILE | S | 39 | 28.357 | 52.161 | 9.336 | 1.00 | 0.00 |
| ATOM | 1656 | C | ILE | S | 39 | 28.315 | 51.748 | 10.797 | 1.00 | 0.00 |
| ATOM | 1657 | O | ILE | S | 39 | 29.332 | 51.467 | 11.425 | 1.00 | 0.00 |
| ATOM | 1658 | CB | ILE | S | 39 | 28.548 | 50.976 | 8.362 | 1.00 | 0.00 |
| ATOM | 1659 | CG1 | ILE | S | 39 | 27.384 | 49.989 | 8.309 | 1.00 | 0.00 |
| ATOM | 1660 | CG2 | ILE | S | 39 | 29.875 | 50.240 | 8.616 | 1.00 | 0.00 |
| ATOM | 1661 | CD1 | ILE | S | 39 | 27.585 | 48.926 | 7.228 | 1.00 | 0.00 |
| ATOM | 1662 | H | ILE | S | 39 | 30.356 | 52.873 | 9.123 | 1.00 | 0.00 |
| ATOM | 1663 | N | SER | S | 40 | 27.089 | 51.627 | 11.287 | 1.00 | 0.00 |
| ATOM | 1664 | CA | SER | S | 40 | 27.013 | 50.865 | 12.528 | 1.00 | 0.00 |
| ATOM | 1665 | C | SER | S | 40 | 26.984 | 49.358 | 12.331 | 1.00 | 0.00 |
| ATOM | 1666 | O | SER | S | 40 | 26.974 | 48.784 | 11.228 | 1.00 | 0.00 |
| ATOM | 1667 | CB | SER | S | 40 | 25.811 | 51.285 | 13.385 | 1.00 | 0.00 |
| ATOM | 1668 | OG | SER | S | 40 | 26.236 | 51.777 | 14.666 | 1.00 | 0.00 |
| ATOM | 1669 | H | SER | S | 40 | 26.287 | 51.895 | 10.758 | 1.00 | 0.00 |
| ATOM | 1670 | HG | SER | S | 40 | 25.552 | 51.470 | 15.275 | 1.00 | 0.00 |
| ATOM | 1671 | N | GLU | S | 41 | 26.933 | 48.774 | 13.534 | 1.00 | 0.00 |
| ATOM | 1672 | CA | GLU | S | 41 | 26.094 | 47.631 | 13.889 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1673 | C | GLU | S | 41 | 24.949 | 47.339 | 12.927 | 1.00 | 0.00 |
| ATOM | 1674 | O | GLU | S | 41 | 24.458 | 48.187 | 12.174 | 1.00 | 0.00 |
| ATOM | 1675 | CB | GLU | S | 41 | 25.549 | 47.936 | 15.284 | 1.00 | 0.00 |
| ATOM | 1676 | CG | GLU | S | 41 | 24.802 | 46.800 | 15.974 | 1.00 | 0.00 |
| ATOM | 1677 | CD | GLU | S | 41 | 23.896 | 47.351 | 17.048 | 1.00 | 0.00 |
| ATOM | 1678 | OE1 | GLU | S | 41 | 23.945 | 46.875 | 18.179 | 1.00 | 0.00 |
| ATOM | 1679 | OE2 | GLU | S | 41 | 23.109 | 48.244 | 16.758 | 1.00 | 0.00 |
| ATOM | 1680 | H | GLU | S | 41 | 27.299 | 49.317 | 14.287 | 1.00 | 0.00 |
| ATOM | 1681 | N | ASN | S | 42 | 24.563 | 46.064 | 12.947 | 1.00 | 0.00 |
| ATOM | 1682 | CA | ASN | S | 42 | 23.217 | 45.700 | 12.522 | 1.00 | 0.00 |
| ATOM | 1683 | C | ASN | S | 42 | 22.472 | 45.227 | 13.759 | 1.00 | 0.00 |
| ATOM | 1684 | O | ASN | S | 42 | 23.031 | 44.495 | 14.586 | 1.00 | 0.00 |
| ATOM | 1685 | CB | ASN | S | 42 | 23.246 | 44.667 | 11.394 | 1.00 | 0.00 |
| ATOM | 1686 | CG | ASN | S | 42 | 23.941 | 43.408 | 11.852 | 1.00 | 0.00 |
| ATOM | 1687 | OD1 | ASN | S | 42 | 25.160 | 43.356 | 12.047 | 1.00 | 0.00 |
| ATOM | 1688 | ND2 | ASN | S | 42 | 23.079 | 42.419 | 12.077 | 1.00 | 0.00 |
| ATOM | 1689 | H | ASN | S | 42 | 25.069 | 45.453 | 13.556 | 1.00 | 0.00 |
| ATOM | 1690 | 1HD2 | ASN | S | 42 | 23.320 | 41.527 | 12.451 | 1.00 | 0.00 |
| ATOM | 1691 | 2HD2 | ASN | S | 42 | 22.108 | 42.552 | 11.856 | 1.00 | 0.00 |
| ATOM | 1692 | N | LYS | S | 43 | 21.256 | 45.763 | 13.906 | 1.00 | 0.00 |
| ATOM | 1693 | CA | LYS | S | 43 | 20.559 | 45.444 | 15.144 | 1.00 | 0.00 |
| ATOM | 1694 | C | LYS | S | 43 | 19.971 | 44.058 | 15.057 | 1.00 | 0.00 |
| ATOM | 1695 | O | LYS | S | 43 | 18.973 | 43.855 | 14.370 | 1.00 | 0.00 |
| ATOM | 1696 | CB | LYS | S | 43 | 19.477 | 46.491 | 15.446 | 1.00 | 0.00 |
| ATOM | 1697 | CG | LYS | S | 43 | 18.605 | 46.212 | 16.685 | 1.00 | 0.00 |
| ATOM | 1698 | CD | LYS | S | 43 | 19.043 | 46.786 | 18.043 | 1.00 | 0.00 |
| ATOM | 1699 | CE | LYS | S | 43 | 20.434 | 46.403 | 18.553 | 1.00 | 0.00 |
| ATOM | 1700 | NZ | LYS | S | 43 | 21.321 | 47.560 | 18.401 | 1.00 | 0.00 |
| ATOM | 1701 | H | LYS | S | 43 | 20.874 | 46.348 | 13.196 | 1.00 | 0.00 |
| ATOM | 1702 | 1HZ | LYS | S | 43 | 22.315 | 47.325 | 18.601 | 1.00 | 0.00 |
| ATOM | 1703 | 2HZ | LYS | S | 43 | 21.391 | 47.873 | 17.411 | 1.00 | 0.00 |
| ATOM | 1704 | 3HZ | LYS | S | 43 | 21.044 | 48.367 | 18.986 | 1.00 | 0.00 |
| ATOM | 1705 | N | THR | S | 44 | 20.650 | 43.162 | 15.783 | 1.00 | 0.00 |
| ATOM | 1706 | CA | THR | S | 44 | 20.305 | 41.743 | 15.796 | 1.00 | 0.00 |
| ATOM | 1707 | C | THR | S | 44 | 20.515 | 41.011 | 14.474 | 1.00 | 0.00 |
| ATOM | 1708 | O | THR | S | 44 | 21.546 | 40.360 | 14.302 | 1.00 | 0.00 |
| ATOM | 1709 | CB | THR | S | 44 | 18.922 | 41.496 | 16.424 | 1.00 | 0.00 |
| ATOM | 1710 | OG1 | THR | S | 44 | 18.836 | 42.143 | 17.710 | 1.00 | 0.00 |
| ATOM | 1711 | CG2 | THR | S | 44 | 18.614 | 40.003 | 16.595 | 1.00 | 0.00 |
| ATOM | 1712 | H | THR | S | 44 | 21.474 | 43.463 | 16.248 | 1.00 | 0.00 |
| ATOM | 1713 | HG1 | THR | S | 44 | 18.041 | 41.760 | 18.074 | 1.00 | 0.00 |
| ATOM | 1714 | N | ASP | S | 45 | 19.529 | 41.116 | 13.580 | 1.00 | 0.00 |
| ATOM | 1715 | CA | ASP | S | 45 | 19.642 | 40.316 | 12.370 | 1.00 | 0.00 |
| ATOM | 1716 | C | ASP | S | 45 | 20.065 | 41.122 | 11.160 | 1.00 | 0.00 |
| ATOM | 1717 | O | ASP | S | 45 | 20.077 | 42.353 | 11.145 | 1.00 | 0.00 |
| ATOM | 1718 | CB | ASP | S | 45 | 18.336 | 39.564 | 12.119 | 1.00 | 0.00 |
| ATOM | 1719 | CG | ASP | S | 45 | 18.662 | 38.134 | 11.743 | 1.00 | 0.00 |
| ATOM | 1720 | OD1 | ASP | S | 45 | 18.512 | 37.258 | 12.592 | 1.00 | 0.00 |
| ATOM | 1721 | OD2 | ASP | S | 45 | 19.070 | 37.896 | 10.607 | 1.00 | 0.00 |
| ATOM | 1722 | H | ASP | S | 45 | 18.791 | 41.772 | 13.716 | 1.00 | 0.00 |
| ATOM | 1723 | N | GLU | S | 46 | 20.427 | 40.393 | 10.105 | 1.00 | 0.00 |
| ATOM | 1724 | CA | GLU | S | 46 | 20.792 | 41.115 | 8.895 | 1.00 | 0.00 |
| ATOM | 1725 | C | GLU | S | 46 | 19.678 | 41.501 | 7.931 | 1.00 | 0.00 |
| ATOM | 1726 | O | GLU | S | 46 | 19.961 | 42.235 | 6.982 | 1.00 | 0.00 |
| ATOM | 1727 | CB | GLU | S | 46 | 21.978 | 40.463 | 8.169 | 1.00 | 0.00 |
| ATOM | 1728 | CG | GLU | S | 46 | 23.363 | 40.819 | 8.752 | 1.00 | 0.00 |
| ATOM | 1729 | CD | GLU | S | 46 | 23.847 | 42.221 | 8.369 | 1.00 | 0.00 |
| ATOM | 1730 | OE1 | GLU | S | 46 | 25.053 | 42.405 | 8.196 | 1.00 | 0.00 |
| ATOM | 1731 | OE2 | GLU | S | 46 | 23.040 | 43.138 | 8.243 | 1.00 | 0.00 |
| ATOM | 1732 | H | GLU | S | 46 | 20.308 | 39.398 | 10.174 | 1.00 | 0.00 |
| ATOM | 1733 | N | GLU | S | 47 | 18.434 | 41.068 | 8.227 | 1.00 | 0.00 |
| ATOM | 1734 | CA | GLU | S | 47 | 17.271 | 41.414 | 7.377 | 1.00 | 0.00 |
| ATOM | 1735 | C | GLU | S | 47 | 17.255 | 42.826 | 6.789 | 1.00 | 0.00 |
| ATOM | 1736 | O | GLU | S | 47 | 17.176 | 43.839 | 7.485 | 1.00 | 0.00 |
| ATOM | 1737 | CB | GLU | S | 47 | 15.935 | 41.145 | 8.092 | 1.00 | 0.00 |
| ATOM | 1738 | CG | GLU | S | 47 | 14.839 | 40.409 | 7.285 | 1.00 | 0.00 |
| ATOM | 1739 | CD | GLU | S | 47 | 14.237 | 41.213 | 6.133 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1740 | OE1 | GLU | S | 47 | 13.183 | 41.822 | 6.300 | 1.00 | 0.00 |
| ATOM | 1741 | OE2 | GLU | S | 47 | 14.796 | 41.211 | 5.041 | 1.00 | 0.00 |
| ATOM | 1742 | H | GLU | S | 47 | 18.333 | 40.428 | 8.991 | 1.00 | 0.00 |
| ATOM | 1743 | N | PRO | S | 48 | 17.419 | 42.856 | 5.448 | 1.00 | 0.00 |
| ATOM | 1744 | CA | PRO | S | 48 | 17.311 | 44.117 | 4.716 | 1.00 | 0.00 |
| ATOM | 1745 | C | PRO | S | 48 | 16.037 | 44.938 | 4.883 | 1.00 | 0.00 |
| ATOM | 1746 | O | PRO | S | 48 | 16.051 | 46.122 | 4.557 | 1.00 | 0.00 |
| ATOM | 1747 | CB | PRO | S | 48 | 17.546 | 43.694 | 3.261 | 1.00 | 0.00 |
| ATOM | 1748 | CG | PRO | S | 48 | 18.367 | 42.410 | 3.346 | 1.00 | 0.00 |
| ATOM | 1749 | CD | PRO | S | 48 | 17.790 | 41.738 | 4.584 | 1.00 | 0.00 |
| ATOM | 1750 | N | GLY | S | 49 | 14.946 | 44.306 | 5.329 | 1.00 | 0.00 |
| ATOM | 1751 | CA | GLY | S | 49 | 13.714 | 45.086 | 5.392 | 1.00 | 0.00 |
| ATOM | 1752 | C | GLY | S | 49 | 13.400 | 45.675 | 6.755 | 1.00 | 0.00 |
| ATOM | 1753 | O | GLY | S | 49 | 13.066 | 46.856 | 6.905 | 1.00 | 0.00 |
| ATOM | 1754 | H | GLY | S | 49 | 14.936 | 43.340 | 5.612 | 1.00 | 0.00 |
| ATOM | 1755 | N | TYR | S | 50 | 13.477 | 44.791 | 7.749 | 1.00 | 0.00 |
| ATOM | 1756 | CA | TYR | S | 50 | 13.077 | 45.223 | 9.084 | 1.00 | 0.00 |
| ATOM | 1757 | C | TYR | S | 50 | 14.172 | 45.896 | 9.893 | 1.00 | 0.00 |
| ATOM | 1758 | O | TYR | S | 50 | 15.332 | 45.502 | 9.876 | 1.00 | 0.00 |
| ATOM | 1759 | CB | TYR | S | 50 | 12.463 | 44.060 | 9.871 | 1.00 | 0.00 |
| ATOM | 1760 | CG | TYR | S | 50 | 10.961 | 44.013 | 9.679 | 1.00 | 0.00 |
| ATOM | 1761 | CD1 | TYR | S | 50 | 10.397 | 43.041 | 8.826 | 1.00 | 0.00 |
| ATOM | 1762 | CD2 | TYR | S | 50 | 10.159 | 44.941 | 10.376 | 1.00 | 0.00 |
| ATOM | 1763 | CE1 | TYR | S | 50 | 8.998 | 42.993 | 8.673 | 1.00 | 0.00 |
| ATOM | 1764 | CE2 | TYR | S | 50 | 8.764 | 44.892 | 10.223 | 1.00 | 0.00 |
| ATOM | 1765 | CZ | TYR | S | 50 | 8.197 | 43.918 | 9.375 | 1.00 | 0.00 |
| ATOM | 1766 | OH | TYR | S | 50 | 6.818 | 43.877 | 9.233 | 1.00 | 0.00 |
| ATOM | 1767 | H | TYR | S | 50 | 13.801 | 43.859 | 7.551 | 1.00 | 0.00 |
| ATOM | 1768 | HH | TYR | S | 50 | 6.436 | 44.530 | 9.805 | 1.00 | 0.00 |
| ATOM | 1769 | N | ILE | S | 51 | 13.709 | 46.933 | 10.625 | 1.00 | 0.00 |
| ATOM | 1770 | CA | ILE | S | 51 | 14.506 | 47.751 | 11.552 | 1.00 | 0.00 |
| ATOM | 1771 | C | ILE | S | 51 | 15.608 | 48.620 | 10.934 | 1.00 | 0.00 |
| ATOM | 1772 | O | ILE | S | 51 | 16.126 | 48.344 | 9.859 | 1.00 | 0.00 |
| ATOM | 1773 | CB | ILE | S | 51 | 14.956 | 46.888 | 12.759 | 1.00 | 0.00 |
| ATOM | 1774 | CG1 | ILE | S | 51 | 14.635 | 47.581 | 14.082 | 1.00 | 0.00 |
| ATOM | 1775 | CG2 | ILE | S | 51 | 16.433 | 46.459 | 12.715 | 1.00 | 0.00 |
| ATOM | 1776 | CD1 | ILE | S | 51 | 14.877 | 46.697 | 15.307 | 1.00 | 0.00 |
| ATOM | 1777 | H | ILE | S | 51 | 12.731 | 47.105 | 10.545 | 1.00 | 0.00 |
| ATOM | 1778 | N | LYS | S | 52 | 15.973 | 49.705 | 11.641 | 1.00 | 0.00 |
| ATOM | 1779 | CA | LYS | S | 52 | 17.127 | 50.472 | 11.165 | 1.00 | 0.00 |
| ATOM | 1780 | C | LYS | S | 52 | 18.440 | 49.892 | 11.666 | 1.00 | 0.00 |
| ATOM | 1781 | O | LYS | S | 52 | 19.155 | 50.432 | 12.509 | 1.00 | 0.00 |
| ATOM | 1782 | CB | LYS | S | 52 | 16.918 | 51.967 | 11.475 | 1.00 | 0.00 |
| ATOM | 1783 | CG | LYS | S | 52 | 18.055 | 53.010 | 11.453 | 1.00 | 0.00 |
| ATOM | 1784 | CD | LYS | S | 52 | 18.818 | 53.181 | 10.141 | 1.00 | 0.00 |
| ATOM | 1785 | CE | LYS | S | 52 | 19.621 | 54.491 | 10.076 | 1.00 | 0.00 |
| ATOM | 1786 | NZ | LYS | S | 52 | 20.680 | 54.588 | 11.081 | 1.00 | 0.00 |
| ATOM | 1787 | H | LYS | S | 52 | 15.607 | 49.877 | 12.558 | 1.00 | 0.00 |
| ATOM | 1788 | 1HZ | LYS | S | 52 | 20.931 | 53.673 | 11.482 | 1.00 | 0.00 |
| ATOM | 1789 | 2HZ | LYS | S | 52 | 21.540 | 55.021 | 10.684 | 1.00 | 0.00 |
| ATOM | 1790 | 3HZ | LYS | S | 52 | 20.370 | 55.187 | 11.867 | 1.00 | 0.00 |
| ATOM | 1791 | N | LYS | S | 53 | 18.759 | 48.769 | 11.010 | 1.00 | 0.00 |
| ATOM | 1792 | CA | LYS | S | 53 | 19.927 | 47.971 | 11.369 | 1.00 | 0.00 |
| ATOM | 1793 | C | LYS | S | 53 | 21.163 | 48.704 | 11.840 | 1.00 | 0.00 |
| ATOM | 1794 | O | LYS | S | 53 | 21.759 | 48.349 | 12.853 | 1.00 | 0.00 |
| ATOM | 1795 | CB | LYS | S | 53 | 20.290 | 47.005 | 10.258 | 1.00 | 0.00 |
| ATOM | 1796 | CG | LYS | S | 53 | 19.231 | 45.924 | 10.065 | 1.00 | 0.00 |
| ATOM | 1797 | CD | LYS | S | 53 | 19.772 | 44.862 | 9.124 | 1.00 | 0.00 |
| ATOM | 1798 | CE | LYS | S | 53 | 20.114 | 45.441 | 7.759 | 1.00 | 0.00 |
| ATOM | 1799 | NZ | LYS | S | 53 | 21.097 | 44.576 | 7.112 | 1.00 | 0.00 |
| ATOM | 1800 | H | LYS | S | 53 | 18.033 | 48.393 | 10.431 | 1.00 | 0.00 |
| ATOM | 1801 | 1HZ | LYS | S | 53 | 20.653 | 43.719 | 6.739 | 1.00 | 0.00 |
| ATOM | 1802 | 2HZ | LYS | S | 53 | 21.561 | 45.094 | 6.352 | 1.00 | 0.00 |
| ATOM | 1803 | 3HZ | LYS | S | 53 | 21.812 | 44.280 | 7.809 | 1.00 | 0.00 |
| ATOM | 1804 | N | CYS | S | 54 | 21.536 | 49.774 | 11.126 | 1.00 | 0.00 |
| ATOM | 1805 | CA | CYS | S | 54 | 22.473 | 50.662 | 11.802 | 1.00 | 0.00 |
| ATOM | 1806 | C | CYS | S | 54 | 21.818 | 51.477 | 12.891 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1807 | O | CYS | S | 54 | 21.392 | 52.600 | 12.635 | 1.00 | 0.00 |
| ATOM | 1808 | CB | CYS | S | 54 | 23.169 | 51.595 | 10.819 | 1.00 | 0.00 |
| ATOM | 1809 | SG | CYS | S | 54 | 24.471 | 50.734 | 9.906 | 1.00 | 0.00 |
| ATOM | 1810 | H | CYS | S | 54 | 21.003 | 49.989 | 10.308 | 1.00 | 0.00 |
| ATOM | 1811 | N | CYS | S | 55 | 21.765 | 50.885 | 14.085 | 1.00 | 0.00 |
| ATOM | 1812 | CA | CYS | S | 55 | 21.492 | 51.763 | 15.218 | 1.00 | 0.00 |
| ATOM | 1813 | C | CYS | S | 55 | 22.721 | 52.610 | 15.429 | 1.00 | 0.00 |
| ATOM | 1814 | O | CYS | S | 55 | 23.745 | 52.150 | 15.937 | 1.00 | 0.00 |
| ATOM | 1815 | CB | CYS | S | 55 | 21.231 | 50.953 | 16.478 | 1.00 | 0.00 |
| ATOM | 1816 | SG | CYS | S | 55 | 19.860 | 49.782 | 16.322 | 1.00 | 0.00 |
| ATOM | 1817 | H | CYS | S | 55 | 22.076 | 49.948 | 14.256 | 1.00 | 0.00 |
| ATOM | 1818 | N | LYS | S | 56 | 22.656 | 53.837 | 14.913 | 1.00 | 0.00 |
| ATOM | 1819 | CA | LYS | S | 56 | 23.995 | 54.399 | 14.851 | 1.00 | 0.00 |
| ATOM | 1820 | C | LYS | S | 56 | 24.307 | 55.314 | 15.993 | 1.00 | 0.00 |
| ATOM | 1821 | O | LYS | S | 56 | 23.440 | 55.932 | 16.613 | 1.00 | 0.00 |
| ATOM | 1822 | CB | LYS | S | 56 | 24.310 | 55.007 | 13.487 | 1.00 | 0.00 |
| ATOM | 1823 | CG | LYS | S | 56 | 25.727 | 54.785 | 12.940 | 1.00 | 0.00 |
| ATOM | 1824 | CD | LYS | S | 56 | 25.996 | 55.352 | 11.538 | 1.00 | 0.00 |
| ATOM | 1825 | CE | LYS | S | 56 | 25.980 | 56.883 | 11.457 | 1.00 | 0.00 |
| ATOM | 1826 | NZ | LYS | S | 56 | 27.073 | 57.393 | 12.270 | 1.00 | 0.00 |
| ATOM | 1827 | H | LYS | S | 56 | 21.817 | 54.307 | 14.651 | 1.00 | 0.00 |
| ATOM | 1828 | 1HZ | LYS | S | 56 | 26.967 | 57.080 | 13.245 | 1.00 | 0.00 |
| ATOM | 1829 | 2HZ | LYS | S | 56 | 27.983 | 57.081 | 11.884 | 1.00 | 0.00 |
| ATOM | 1830 | 3HZ | LYS | S | 56 | 27.157 | 58.420 | 12.192 | 1.00 | 0.00 |
| ATOM | 1831 | N | GLY | S | 57 | 25.614 | 55.306 | 16.278 | 1.00 | 0.00 |
| ATOM | 1832 | CA | GLY | S | 57 | 26.202 | 56.429 | 16.983 | 1.00 | 0.00 |
| ATOM | 1833 | C | GLY | S | 57 | 27.113 | 57.120 | 15.998 | 1.00 | 0.00 |
| ATOM | 1834 | O | GLY | S | 57 | 27.257 | 56.728 | 14.830 | 1.00 | 0.00 |
| ATOM | 1835 | H | GLY | S | 57 | 26.209 | 54.699 | 15.751 | 1.00 | 0.00 |
| ATOM | 1836 | N | PHE | S | 58 | 27.742 | 58.180 | 16.473 | 1.00 | 0.00 |
| ATOM | 1837 | CA | PHE | S | 58 | 28.591 | 58.838 | 15.490 | 1.00 | 0.00 |
| ATOM | 1838 | C | PHE | S | 58 | 30.081 | 58.528 | 15.560 | 1.00 | 0.00 |
| ATOM | 1839 | O | PHE | S | 58 | 30.868 | 58.834 | 14.663 | 1.00 | 0.00 |
| ATOM | 1840 | CB | PHE | S | 58 | 28.223 | 60.320 | 15.411 | 1.00 | 0.00 |
| ATOM | 1841 | CG | PHE | S | 58 | 26.841 | 60.454 | 14.806 | 1.00 | 0.00 |
| ATOM | 1842 | CD1 | PHE | S | 58 | 25.703 | 60.480 | 15.642 | 1.00 | 0.00 |
| ATOM | 1843 | CD2 | PHE | S | 58 | 26.705 | 60.524 | 13.404 | 1.00 | 0.00 |
| ATOM | 1844 | CE1 | PHE | S | 58 | 24.416 | 60.545 | 15.076 | 1.00 | 0.00 |
| ATOM | 1845 | CE2 | PHE | S | 58 | 25.420 | 60.586 | 12.833 | 1.00 | 0.00 |
| ATOM | 1846 | CZ | PHE | S | 58 | 24.287 | 60.589 | 13.673 | 1.00 | 0.00 |
| ATOM | 1847 | H | PHE | S | 58 | 27.581 | 58.485 | 17.409 | 1.00 | 0.00 |
| ATOM | 1848 | N | CYS | S | 59 | 30.478 | 57.826 | 16.642 | 1.00 | 0.00 |
| ATOM | 1849 | CA | CYS | S | 59 | 31.859 | 57.324 | 16.732 | 1.00 | 0.00 |
| ATOM | 1850 | C | CYS | S | 59 | 32.192 | 56.338 | 15.628 | 1.00 | 0.00 |
| ATOM | 1851 | O | CYS | S | 59 | 33.182 | 56.455 | 14.900 | 1.00 | 0.00 |
| ATOM | 1852 | CB | CYS | S | 59 | 32.153 | 56.701 | 18.096 | 1.00 | 0.00 |
| ATOM | 1853 | SG | CYS | S | 59 | 33.930 | 56.457 | 18.379 | 1.00 | 0.00 |
| ATOM | 1854 | H | CYS | S | 59 | 29.761 | 57.539 | 17.274 | 1.00 | 0.00 |
| ATOM | 1855 | N | ILE | S | 60 | 31.196 | 55.465 | 15.429 | 1.00 | 0.00 |
| ATOM | 1856 | CA | ILE | S | 60 | 31.219 | 54.668 | 14.201 | 1.00 | 0.00 |
| ATOM | 1857 | C | ILE | S | 60 | 31.218 | 55.417 | 12.869 | 1.00 | 0.00 |
| ATOM | 1858 | O | ILE | S | 60 | 30.907 | 54.805 | 11.848 | 1.00 | 0.00 |
| ATOM | 1859 | CB | ILE | S | 60 | 30.094 | 53.613 | 14.127 | 1.00 | 0.00 |
| ATOM | 1860 | CG1 | ILE | S | 60 | 28.818 | 53.875 | 14.936 | 1.00 | 0.00 |
| ATOM | 1861 | CG2 | ILE | S | 60 | 30.644 | 52.208 | 14.372 | 1.00 | 0.00 |
| ATOM | 1862 | CD1 | ILE | S | 60 | 28.838 | 53.453 | 16.409 | 1.00 | 0.00 |
| ATOM | 1863 | H | ILE | S | 60 | 30.376 | 55.530 | 15.995 | 1.00 | 0.00 |
| ATOM | 1864 | N | ASP | S | 61 | 31.544 | 56.732 | 12.867 | 1.00 | 0.00 |
| ATOM | 1865 | CA | ASP | S | 61 | 31.852 | 57.492 | 11.650 | 1.00 | 0.00 |
| ATOM | 1866 | C | ASP | S | 61 | 33.298 | 57.956 | 11.497 | 1.00 | 0.00 |
| ATOM | 1867 | O | ASP | S | 61 | 33.756 | 58.269 | 10.394 | 1.00 | 0.00 |
| ATOM | 1868 | CB | ASP | S | 61 | 30.960 | 58.722 | 11.484 | 1.00 | 0.00 |
| ATOM | 1869 | CG | ASP | S | 61 | 29.530 | 58.403 | 11.109 | 1.00 | 0.00 |
| ATOM | 1870 | OD1 | ASP | S | 61 | 28.655 | 59.198 | 11.420 | 1.00 | 0.00 |
| ATOM | 1871 | OD2 | ASP | S | 61 | 29.253 | 57.372 | 10.509 | 1.00 | 0.00 |
| ATOM | 1872 | H | ASP | S | 61 | 31.691 | 57.209 | 13.731 | 1.00 | 0.00 |
| ATOM | 1873 | N | ILE | S | 62 | 34.058 | 57.953 | 12.606 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1874 | CA | ILE | S | 62 | 35.496 | 58.271 | 12.580 | 1.00 | 0.00 |
| ATOM | 1875 | C | ILE | S | 62 | 36.340 | 57.299 | 11.744 | 1.00 | 0.00 |
| ATOM | 1876 | O | ILE | S | 62 | 37.488 | 57.512 | 11.358 | 1.00 | 0.00 |
| ATOM | 1877 | CB | ILE | S | 62 | 36.024 | 58.411 | 14.015 | 1.00 | 0.00 |
| ATOM | 1878 | CG1 | ILE | S | 62 | 35.070 | 59.286 | 14.830 | 1.00 | 0.00 |
| ATOM | 1879 | CG2 | ILE | S | 62 | 37.427 | 59.030 | 14.039 | 1.00 | 0.00 |
| ATOM | 1880 | CD1 | ILE | S | 62 | 35.288 | 59.125 | 16.328 | 1.00 | 0.00 |
| ATOM | 1881 | H | ILE | S | 62 | 33.567 | 57.803 | 13.459 | 1.00 | 0.00 |
| ATOM | 1882 | N | LEU | S | 63 | 35.637 | 56.233 | 11.359 | 1.00 | 0.00 |
| ATOM | 1883 | CA | LEU | S | 63 | 36.072 | 55.418 | 10.227 | 1.00 | 0.00 |
| ATOM | 1884 | C | LEU | S | 63 | 36.195 | 56.140 | 8.868 | 1.00 | 0.00 |
| ATOM | 1885 | O | LEU | S | 63 | 36.594 | 55.566 | 7.865 | 1.00 | 0.00 |
| ATOM | 1886 | CB | LEU | S | 63 | 35.164 | 54.192 | 10.150 | 1.00 | 0.00 |
| ATOM | 1887 | CG | LEU | S | 63 | 34.839 | 53.535 | 11.499 | 1.00 | 0.00 |
| ATOM | 1888 | CD1 | LEU | S | 63 | 33.760 | 52.462 | 11.356 | 1.00 | 0.00 |
| ATOM | 1889 | CD2 | LEU | S | 63 | 36.083 | 53.021 | 12.225 | 1.00 | 0.00 |
| ATOM | 1890 | H | LEU | S | 63 | 34.750 | 56.114 | 11.806 | 1.00 | 0.00 |
| ATOM | 1891 | N | LYS | S | 64 | 35.891 | 57.451 | 8.864 | 1.00 | 0.00 |
| ATOM | 1892 | CA | LYS | S | 64 | 36.354 | 58.311 | 7.780 | 1.00 | 0.00 |
| ATOM | 1893 | C | LYS | S | 64 | 37.874 | 58.346 | 7.711 | 1.00 | 0.00 |
| ATOM | 1894 | O | LYS | S | 64 | 38.466 | 57.840 | 6.775 | 1.00 | 0.00 |
| ATOM | 1895 | CB | LYS | S | 64 | 35.700 | 59.686 | 7.946 | 1.00 | 0.00 |
| ATOM | 1896 | CG | LYS | S | 64 | 35.934 | 60.695 | 6.822 | 1.00 | 0.00 |
| ATOM | 1897 | CD | LYS | S | 64 | 36.915 | 61.798 | 7.218 | 1.00 | 0.00 |
| ATOM | 1898 | CE | LYS | S | 64 | 37.026 | 62.857 | 6.126 | 1.00 | 0.00 |
| ATOM | 1899 | NZ | LYS | S | 64 | 37.892 | 63.948 | 6.577 | 1.00 | 0.00 |
| ATOM | 1900 | H | LYS | S | 64 | 35.455 | 57.815 | 9.679 | 1.00 | 0.00 |
| ATOM | 1901 | 1HZ | LYS | S | 64 | 37.857 | 64.705 | 5.877 | 1.00 | 0.00 |
| ATOM | 1902 | 2HZ | LYS | S | 64 | 37.597 | 64.392 | 7.464 | 1.00 | 0.00 |
| ATOM | 1903 | 3HZ | LYS | S | 64 | 38.895 | 63.681 | 6.624 | 1.00 | 0.00 |
| ATOM | 1904 | N | LYS | S | 65 | 38.494 | 58.887 | 8.773 | 1.00 | 0.00 |
| ATOM | 1905 | CA | LYS | S | 65 | 39.953 | 58.831 | 8.736 | 1.00 | 0.00 |
| ATOM | 1906 | C | LYS | S | 65 | 40.567 | 57.450 | 8.957 | 1.00 | 0.00 |
| ATOM | 1907 | O | LYS | S | 65 | 41.660 | 57.159 | 8.482 | 1.00 | 0.00 |
| ATOM | 1908 | CB | LYS | S | 65 | 40.523 | 59.909 | 9.669 | 1.00 | 0.00 |
| ATOM | 1909 | CG | LYS | S | 65 | 42.023 | 60.205 | 9.515 | 1.00 | 0.00 |
| ATOM | 1910 | CD | LYS | S | 65 | 42.470 | 60.546 | 8.085 | 1.00 | 0.00 |
| ATOM | 1911 | CE | LYS | S | 65 | 41.774 | 61.751 | 7.440 | 1.00 | 0.00 |
| ATOM | 1912 | NZ | LYS | S | 65 | 42.195 | 63.033 | 8.022 | 1.00 | 0.00 |
| ATOM | 1913 | H | LYS | S | 65 | 37.974 | 59.217 | 9.563 | 1.00 | 0.00 |
| ATOM | 1914 | 1HZ | LYS | S | 65 | 43.176 | 63.269 | 7.774 | 1.00 | 0.00 |
| ATOM | 1915 | 2HZ | LYS | S | 65 | 41.595 | 63.799 | 7.662 | 1.00 | 0.00 |
| ATOM | 1916 | 3HZ | LYS | S | 65 | 42.124 | 63.051 | 9.062 | 1.00 | 0.00 |
| ATOM | 1917 | N | ILE | S | 66 | 39.827 | 56.621 | 9.707 | 1.00 | 0.00 |
| ATOM | 1918 | CA | ILE | S | 66 | 40.422 | 55.343 | 10.089 | 1.00 | 0.00 |
| ATOM | 1919 | C | ILE | S | 66 | 39.666 | 54.090 | 9.624 | 1.00 | 0.00 |
| ATOM | 1920 | O | ILE | S | 66 | 39.784 | 52.983 | 10.162 | 1.00 | 0.00 |
| ATOM | 1921 | CB | ILE | S | 66 | 40.758 | 55.411 | 11.591 | 1.00 | 0.00 |
| ATOM | 1922 | CG1 | ILE | S | 66 | 42.091 | 54.760 | 12.003 | 1.00 | 0.00 |
| ATOM | 1923 | CG2 | ILE | S | 66 | 39.564 | 54.996 | 12.463 | 1.00 | 0.00 |
| ATOM | 1924 | CD1 | ILE | S | 66 | 42.258 | 53.243 | 11.869 | 1.00 | 0.00 |
| ATOM | 1925 | H | ILE | S | 66 | 38.911 | 56.863 | 10.016 | 1.00 | 0.00 |
| ATOM | 1926 | N | SER | S | 67 | 38.905 | 54.324 | 8.548 | 1.00 | 0.00 |
| ATOM | 1927 | CA | SER | S | 67 | 38.711 | 53.250 | 7.584 | 1.00 | 0.00 |
| ATOM | 1928 | C | SER | S | 67 | 39.010 | 53.712 | 6.170 | 1.00 | 0.00 |
| ATOM | 1929 | O | SER | S | 67 | 40.071 | 53.409 | 5.626 | 1.00 | 0.00 |
| ATOM | 1930 | CB | SER | S | 67 | 37.329 | 52.574 | 7.620 | 1.00 | 0.00 |
| ATOM | 1931 | OG | SER | S | 67 | 37.056 | 51.933 | 8.875 | 1.00 | 0.00 |
| ATOM | 1932 | H | SER | S | 67 | 38.662 | 55.255 | 8.294 | 1.00 | 0.00 |
| ATOM | 1933 | HG | SER | S | 67 | 37.868 | 51.462 | 9.099 | 1.00 | 0.00 |
| ATOM | 1934 | N | LYS | S | 68 | 38.020 | 54.414 | 5.583 | 1.00 | 0.00 |
| ATOM | 1935 | CA | LYS | S | 68 | 37.880 | 54.491 | 4.123 | 1.00 | 0.00 |
| ATOM | 1936 | C | LYS | S | 68 | 39.156 | 54.544 | 3.294 | 1.00 | 0.00 |
| ATOM | 1937 | O | LYS | S | 68 | 39.326 | 53.859 | 2.284 | 1.00 | 0.00 |
| ATOM | 1938 | CB | LYS | S | 68 | 36.928 | 55.633 | 3.746 | 1.00 | 0.00 |
| ATOM | 1939 | CG | LYS | S | 68 | 35.531 | 55.428 | 4.342 | 1.00 | 0.00 |
| ATOM | 1940 | CD | LYS | S | 68 | 34.492 | 56.473 | 3.925 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1941 | CE | LYS | S | 68 | 33.127 | 56.122 | 4.518 | 1.00 | 0.00 |
| ATOM | 1942 | NZ | LYS | S | 68 | 32.076 | 57.027 | 4.043 | 1.00 | 0.00 |
| ATOM | 1943 | H | LYS | S | 68 | 37.341 | 54.831 | 6.185 | 1.00 | 0.00 |
| ATOM | 1944 | 1HZ | LYS | S | 68 | 31.156 | 56.671 | 4.351 | 1.00 | 0.00 |
| ATOM | 1945 | 2HZ | LYS | S | 68 | 32.151 | 57.989 | 4.424 | 1.00 | 0.00 |
| ATOM | 1946 | 3HZ | LYS | S | 68 | 32.042 | 57.100 | 3.008 | 1.00 | 0.00 |
| ATOM | 1947 | N | SER | S | 69 | 40.065 | 55.396 | 3.774 | 1.00 | 0.00 |
| ATOM | 1948 | CA | SER | S | 69 | 41.322 | 55.450 | 3.041 | 1.00 | 0.00 |
| ATOM | 1949 | C | SER | S | 69 | 42.542 | 54.738 | 3.613 | 1.00 | 0.00 |
| ATOM | 1950 | O | SER | S | 69 | 43.448 | 54.379 | 2.872 | 1.00 | 0.00 |
| ATOM | 1951 | CB | SER | S | 69 | 41.630 | 56.899 | 2.686 | 1.00 | 0.00 |
| ATOM | 1952 | OG | SER | S | 69 | 40.435 | 57.512 | 2.164 | 1.00 | 0.00 |
| ATOM | 1953 | H | SER | S | 69 | 39.822 | 55.929 | 4.586 | 1.00 | 0.00 |
| ATOM | 1954 | HG | SER | S | 69 | 40.399 | 57.215 | 1.254 | 1.00 | 0.00 |
| ATOM | 1955 | N | VAL | S | 70 | 42.601 | 54.547 | 4.947 | 1.00 | 0.00 |
| ATOM | 1956 | CA | VAL | S | 70 | 43.942 | 54.229 | 5.462 | 1.00 | 0.00 |
| ATOM | 1957 | C | VAL | S | 70 | 44.476 | 52.827 | 5.149 | 1.00 | 0.00 |
| ATOM | 1958 | O | VAL | S | 70 | 45.528 | 52.656 | 4.543 | 1.00 | 0.00 |
| ATOM | 1959 | CB | VAL | S | 70 | 44.102 | 54.658 | 6.938 | 1.00 | 0.00 |
| ATOM | 1960 | CG1 | VAL | S | 70 | 43.087 | 54.010 | 7.874 | 1.00 | 0.00 |
| ATOM | 1961 | CG2 | VAL | S | 70 | 45.544 | 54.497 | 7.429 | 1.00 | 0.00 |
| ATOM | 1962 | H | VAL | S | 70 | 41.770 | 54.592 | 5.510 | 1.00 | 0.00 |
| ATOM | 1963 | N | LYS | S | 71 | 43.690 | 51.808 | 5.499 | 1.00 | 0.00 |
| ATOM | 1964 | CA | LYS | S | 71 | 44.046 | 50.563 | 4.828 | 1.00 | 0.00 |
| ATOM | 1965 | C | LYS | S | 71 | 43.308 | 50.461 | 3.503 | 1.00 | 0.00 |
| ATOM | 1966 | O | LYS | S | 71 | 42.248 | 49.869 | 3.376 | 1.00 | 0.00 |
| ATOM | 1967 | CB | LYS | S | 71 | 43.858 | 49.373 | 5.782 | 1.00 | 0.00 |
| ATOM | 1968 | CG | LYS | S | 71 | 44.307 | 48.007 | 5.254 | 1.00 | 0.00 |
| ATOM | 1969 | CD | LYS | S | 71 | 44.359 | 46.943 | 6.357 | 1.00 | 0.00 |
| ATOM | 1970 | CE | LYS | S | 71 | 44.691 | 45.543 | 5.829 | 1.00 | 0.00 |
| ATOM | 1971 | NZ | LYS | S | 71 | 45.171 | 44.696 | 6.930 | 1.00 | 0.00 |
| ATOM | 1972 | H | LYS | S | 71 | 42.841 | 51.884 | 6.031 | 1.00 | 0.00 |
| ATOM | 1973 | 1HZ | LYS | S | 71 | 46.106 | 45.031 | 7.255 | 1.00 | 0.00 |
| ATOM | 1974 | 2HZ | LYS | S | 71 | 44.493 | 44.713 | 7.719 | 1.00 | 0.00 |
| ATOM | 1975 | 3HZ | LYS | S | 71 | 45.306 | 43.707 | 6.649 | 1.00 | 0.00 |
| ATOM | 1976 | N | PHE | S | 72 | 43.917 | 51.105 | 2.476 | 1.00 | 0.00 |
| ATOM | 1977 | CA | PHE | S | 72 | 43.299 | 51.131 | 1.136 | 1.00 | 0.00 |
| ATOM | 1978 | C | PHE | S | 72 | 42.816 | 49.751 | 0.719 | 1.00 | 0.00 |
| ATOM | 1979 | O | PHE | S | 72 | 41.671 | 49.518 | 0.359 | 1.00 | 0.00 |
| ATOM | 1980 | CB | PHE | S | 72 | 44.283 | 51.643 | 0.075 | 1.00 | 0.00 |
| ATOM | 1981 | CG | PHE | S | 72 | 44.685 | 53.081 | 0.308 | 1.00 | 0.00 |
| ATOM | 1982 | CD1 | PHE | S | 72 | 45.857 | 53.367 | 1.044 | 1.00 | 0.00 |
| ATOM | 1983 | CD2 | PHE | S | 72 | 43.889 | 54.117 | -0.229 | 1.00 | 0.00 |
| ATOM | 1984 | CE1 | PHE | S | 72 | 46.240 | 54.707 | 1.245 | 1.00 | 0.00 |
| ATOM | 1985 | CE2 | PHE | S | 72 | 44.272 | 55.458 | -0.031 | 1.00 | 0.00 |
| ATOM | 1986 | CZ | PHE | S | 72 | 45.444 | 55.739 | 0.703 | 1.00 | 0.00 |
| ATOM | 1987 | H | PHE | S | 72 | 44.694 | 51.687 | 2.725 | 1.00 | 0.00 |
| ATOM | 1988 | N | THR | S | 73 | 43.789 | 48.848 | 0.925 | 1.00 | 0.00 |
| ATOM | 1989 | CA | THR | S | 73 | 43.629 | 47.402 | 0.812 | 1.00 | 0.00 |
| ATOM | 1990 | C | THR | S | 73 | 42.765 | 46.724 | 1.878 | 1.00 | 0.00 |
| ATOM | 1991 | O | THR | S | 73 | 43.200 | 45.773 | 2.523 | 1.00 | 0.00 |
| ATOM | 1992 | CB | THR | S | 73 | 45.042 | 46.785 | 0.727 | 1.00 | 0.00 |
| ATOM | 1993 | OG1 | THR | S | 73 | 44.989 | 45.366 | 0.568 | 1.00 | 0.00 |
| ATOM | 1994 | CG2 | THR | S | 73 | 45.959 | 47.162 | 1.899 | 1.00 | 0.00 |
| ATOM | 1995 | H | THR | S | 73 | 44.648 | 49.225 | 1.263 | 1.00 | 0.00 |
| ATOM | 1996 | HG1 | THR | S | 73 | 44.616 | 45.037 | 1.393 | 1.00 | 0.00 |
| ATOM | 1997 | N | TYR | S | 74 | 41.520 | 47.220 | 1.946 | 1.00 | 0.00 |
| ATOM | 1998 | CA | TYR | S | 74 | 40.488 | 46.787 | 2.891 | 1.00 | 0.00 |
| ATOM | 1999 | C | TYR | S | 74 | 40.651 | 47.285 | 4.324 | 1.00 | 0.00 |
| ATOM | 2000 | O | TYR | S | 74 | 41.164 | 46.614 | 5.212 | 1.00 | 0.00 |
| ATOM | 2001 | CB | TYR | S | 74 | 40.196 | 45.270 | 2.842 | 1.00 | 0.00 |
| ATOM | 2002 | CG | TYR | S | 74 | 40.053 | 44.735 | 1.425 | 1.00 | 0.00 |
| ATOM | 2003 | CD1 | TYR | S | 74 | 40.888 | 43.670 | 1.023 | 1.00 | 0.00 |
| ATOM | 2004 | CD2 | TYR | S | 74 | 39.097 | 45.288 | 0.547 | 1.00 | 0.00 |
| ATOM | 2005 | CE1 | TYR | S | 74 | 40.761 | 43.142 | -0.275 | 1.00 | 0.00 |
| ATOM | 2006 | CE2 | TYR | S | 74 | 38.976 | 44.766 | -0.754 | 1.00 | 0.00 |
| ATOM | 2007 | CZ | TYR | S | 74 | 39.807 | 43.697 | -1.152 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2008 | OH | TYR | S | 74 | 39.680 | 43.188 | -2.439 | 1.00 | 0.00 |
| ATOM | 2009 | H | TYR | S | 74 | 41.301 | 47.970 | 1.326 | 1.00 | 0.00 |
| ATOM | 2010 | HH | TYR | S | 74 | 39.485 | 43.914 | -3.020 | 1.00 | 0.00 |
| ATOM | 2011 | N | ASP | S | 75 | 40.130 | 48.507 | 4.520 | 1.00 | 0.00 |
| ATOM | 2012 | CA | ASP | S | 75 | 39.808 | 48.925 | 5.887 | 1.00 | 0.00 |
| ATOM | 2013 | C | ASP | S | 75 | 38.309 | 48.945 | 6.087 | 1.00 | 0.00 |
| ATOM | 2014 | O | ASP | S | 75 | 37.536 | 49.635 | 5.411 | 1.00 | 0.00 |
| ATOM | 2015 | CB | ASP | S | 75 | 40.418 | 50.284 | 6.246 | 1.00 | 0.00 |
| ATOM | 2016 | CG | ASP | S | 75 | 40.537 | 50.543 | 7.752 | 1.00 | 0.00 |
| ATOM | 2017 | OD1 | ASP | S | 75 | 39.767 | 50.011 | 8.554 | 1.00 | 0.00 |
| ATOM | 2018 | OD2 | ASP | S | 75 | 41.412 | 51.316 | 8.135 | 1.00 | 0.00 |
| ATOM | 2019 | H | ASP | S | 75 | 39.894 | 49.099 | 3.752 | 1.00 | 0.00 |
| ATOM | 2020 | N | LEU | S | 76 | 37.951 | 48.062 | 7.019 | 1.00 | 0.00 |
| ATOM | 2021 | CA | LEU | S | 76 | 36.542 | 47.886 | 7.299 | 1.00 | 0.00 |
| ATOM | 2022 | C | LEU | S | 76 | 36.424 | 47.455 | 8.736 | 1.00 | 0.00 |
| ATOM | 2023 | O | LEU | S | 76 | 37.285 | 46.747 | 9.261 | 1.00 | 0.00 |
| ATOM | 2024 | CB | LEU | S | 76 | 35.928 | 46.864 | 6.332 | 1.00 | 0.00 |
| ATOM | 2025 | CG | LEU | S | 76 | 34.402 | 46.744 | 6.410 | 1.00 | 0.00 |
| ATOM | 2026 | CD1 | LEU | S | 76 | 33.698 | 48.055 | 6.049 | 1.00 | 0.00 |
| ATOM | 2027 | CD2 | LEU | S | 76 | 33.886 | 45.564 | 5.587 | 1.00 | 0.00 |
| ATOM | 2028 | H | LEU | S | 76 | 38.643 | 47.644 | 7.609 | 1.00 | 0.00 |
| ATOM | 2029 | N | TYR | S | 77 | 35.325 | 47.933 | 9.341 | 1.00 | 0.00 |
| ATOM | 2030 | CA | TYR | S | 77 | 35.061 | 47.558 | 10.725 | 1.00 | 0.00 |
| ATOM | 2031 | C | TYR | S | 77 | 33.813 | 46.702 | 10.844 | 1.00 | 0.00 |
| ATOM | 2032 | O | TYR | S | 77 | 32.685 | 47.112 | 10.536 | 1.00 | 0.00 |
| ATOM | 2033 | CB | TYR | S | 77 | 34.946 | 48.805 | 11.607 | 1.00 | 0.00 |
| ATOM | 2034 | CG | TYR | S | 77 | 36.296 | 49.301 | 12.086 | 1.00 | 0.00 |
| ATOM | 2035 | CD1 | TYR | S | 77 | 36.511 | 49.350 | 13.477 | 1.00 | 0.00 |
| ATOM | 2036 | CD2 | TYR | S | 77 | 37.290 | 49.716 | 11.171 | 1.00 | 0.00 |
| ATOM | 2037 | CE1 | TYR | S | 77 | 37.736 | 49.828 | 13.968 | 1.00 | 0.00 |
| ATOM | 2038 | CE2 | TYR | S | 77 | 38.520 | 50.192 | 11.660 | 1.00 | 0.00 |
| ATOM | 2039 | CZ | TYR | S | 77 | 38.727 | 50.239 | 13.055 | 1.00 | 0.00 |
| ATOM | 2040 | OH | TYR | S | 77 | 39.927 | 50.691 | 13.575 | 1.00 | 0.00 |
| ATOM | 2041 | H | TYR | S | 77 | 34.713 | 48.537 | 8.839 | 1.00 | 0.00 |
| ATOM | 2042 | HH | TYR | S | 77 | 40.507 | 50.842 | 12.826 | 1.00 | 0.00 |
| ATOM | 2043 | N | LEU | S | 78 | 34.078 | 45.477 | 11.314 | 1.00 | 0.00 |
| ATOM | 2044 | CA | LEU | S | 78 | 32.970 | 44.525 | 11.354 | 1.00 | 0.00 |
| ATOM | 2045 | C | LEU | S | 78 | 32.020 | 44.622 | 12.550 | 1.00 | 0.00 |
| ATOM | 2046 | O | LEU | S | 78 | 31.225 | 43.722 | 12.829 | 1.00 | 0.00 |
| ATOM | 2047 | CB | LEU | S | 78 | 33.511 | 43.109 | 11.142 | 1.00 | 0.00 |
| ATOM | 2048 | CG | LEU | S | 78 | 32.539 | 42.176 | 10.413 | 1.00 | 0.00 |
| ATOM | 2049 | CD1 | LEU | S | 78 | 32.153 | 42.716 | 9.034 | 1.00 | 0.00 |
| ATOM | 2050 | CD2 | LEU | S | 78 | 33.081 | 40.749 | 10.337 | 1.00 | 0.00 |
| ATOM | 2051 | H | LEU | S | 78 | 35.019 | 45.229 | 11.554 | 1.00 | 0.00 |
| ATOM | 2052 | N | VAL | S | 79 | 32.099 | 45.784 | 13.237 | 1.00 | 0.00 |
| ATOM | 2053 | CA | VAL | S | 79 | 31.228 | 46.163 | 14.364 | 1.00 | 0.00 |
| ATOM | 2054 | C | VAL | S | 79 | 29.849 | 45.510 | 14.450 | 1.00 | 0.00 |
| ATOM | 2055 | O | VAL | S | 79 | 28.885 | 46.029 | 13.887 | 1.00 | 0.00 |
| ATOM | 2056 | CB | VAL | S | 79 | 31.128 | 47.709 | 14.418 | 1.00 | 0.00 |
| ATOM | 2057 | CG1 | VAL | S | 79 | 30.710 | 48.343 | 13.085 | 1.00 | 0.00 |
| ATOM | 2058 | CG2 | VAL | S | 79 | 30.300 | 48.202 | 15.613 | 1.00 | 0.00 |
| ATOM | 2059 | H | VAL | S | 79 | 32.785 | 46.430 | 12.905 | 1.00 | 0.00 |
| ATOM | 2060 | N | THR | S | 80 | 29.759 | 44.362 | 15.137 | 1.00 | 0.00 |
| ATOM | 2061 | CA | THR | S | 80 | 28.472 | 43.657 | 15.092 | 1.00 | 0.00 |
| ATOM | 2062 | C | THR | S | 80 | 28.129 | 42.800 | 16.311 | 1.00 | 0.00 |
| ATOM | 2063 | O | THR | S | 80 | 27.025 | 42.894 | 16.845 | 1.00 | 0.00 |
| ATOM | 2064 | CB | THR | S | 80 | 28.308 | 42.876 | 13.752 | 1.00 | 0.00 |
| ATOM | 2065 | OG1 | THR | S | 80 | 27.965 | 43.767 | 12.668 | 1.00 | 0.00 |
| ATOM | 2066 | CG2 | THR | S | 80 | 27.295 | 41.722 | 13.784 | 1.00 | 0.00 |
| ATOM | 2067 | H | THR | S | 80 | 30.575 | 44.069 | 15.643 | 1.00 | 0.00 |
| ATOM | 2068 | HG1 | THR | S | 80 | 27.009 | 43.703 | 12.585 | 1.00 | 0.00 |
| ATOM | 2069 | N | ASN | S | 81 | 29.065 | 41.915 | 16.693 | 1.00 | 0.00 |
| ATOM | 2070 | CA | ASN | S | 81 | 28.573 | 40.849 | 17.582 | 1.00 | 0.00 |
| ATOM | 2071 | C | ASN | S | 81 | 28.799 | 41.169 | 19.048 | 1.00 | 0.00 |
| ATOM | 2072 | O | ASN | S | 81 | 29.425 | 40.445 | 19.823 | 1.00 | 0.00 |
| ATOM | 2073 | CB | ASN | S | 81 | 29.160 | 39.484 | 17.168 | 1.00 | 0.00 |
| ATOM | 2074 | CG | ASN | S | 81 | 28.536 | 38.298 | 17.909 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2075 | OD1 | ASN | S | 81 | 28.817 | 38.023 | 19.077 | 1.00 | 0.00 |
| ATOM | 2076 | ND2 | ASN | S | 81 | 27.751 | 37.517 | 17.158 | 1.00 | 0.00 |
| ATOM | 2077 | H | ASN | S | 81 | 30.038 | 41.988 | 16.473 | 1.00 | 0.00 |
| ATOM | 2078 | 1HD2 | ASN | S | 81 | 27.297 | 36.718 | 17.545 | 1.00 | 0.00 |
| ATOM | 2079 | 2HD2 | ASN | S | 81 | 27.640 | 37.691 | 16.181 | 1.00 | 0.00 |
| ATOM | 2080 | N | GLY | S | 82 | 28.297 | 42.339 | 19.437 | 1.00 | 0.00 |
| ATOM | 2081 | CA | GLY | S | 82 | 28.789 | 42.765 | 20.738 | 1.00 | 0.00 |
| ATOM | 2082 | C | GLY | S | 82 | 27.848 | 42.677 | 21.896 | 1.00 | 0.00 |
| ATOM | 2083 | O | GLY | S | 82 | 28.002 | 41.892 | 22.824 | 1.00 | 0.00 |
| ATOM | 2084 | H | GLY | S | 82 | 27.810 | 42.910 | 18.773 | 1.00 | 0.00 |
| ATOM | 2085 | N | LYS | S | 83 | 26.857 | 43.576 | 21.784 | 1.00 | 0.00 |
| ATOM | 2086 | CA | LYS | S | 83 | 25.787 | 43.774 | 22.760 | 1.00 | 0.00 |
| ATOM | 2087 | C | LYS | S | 83 | 26.200 | 43.663 | 24.222 | 1.00 | 0.00 |
| ATOM | 2088 | O | LYS | S | 83 | 25.548 | 43.078 | 25.085 | 1.00 | 0.00 |
| ATOM | 2089 | CB | LYS | S | 83 | 24.535 | 42.979 | 22.356 | 1.00 | 0.00 |
| ATOM | 2090 | CG | LYS | S | 83 | 24.014 | 43.380 | 20.958 | 1.00 | 0.00 |
| ATOM | 2091 | CD | LYS | S | 83 | 24.650 | 42.620 | 19.780 | 1.00 | 0.00 |
| ATOM | 2092 | CE | LYS | S | 83 | 24.346 | 43.191 | 18.390 | 1.00 | 0.00 |
| ATOM | 2093 | NZ | LYS | S | 83 | 25.141 | 44.389 | 18.097 | 1.00 | 0.00 |
| ATOM | 2094 | H | LYS | S | 83 | 26.866 | 44.119 | 20.944 | 1.00 | 0.00 |
| ATOM | 2095 | 1HZ | LYS | S | 83 | 24.521 | 45.193 | 17.870 | 1.00 | 0.00 |
| ATOM | 2096 | 2HZ | LYS | S | 83 | 25.746 | 44.679 | 18.891 | 1.00 | 0.00 |
| ATOM | 2097 | 3HZ | LYS | S | 83 | 25.750 | 44.229 | 17.268 | 1.00 | 0.00 |
| ATOM | 2098 | N | HIS | S | 84 | 27.360 | 44.316 | 24.450 | 1.00 | 0.00 |
| ATOM | 2099 | CA | HIS | S | 84 | 28.034 | 44.365 | 25.749 | 1.00 | 0.00 |
| ATOM | 2100 | C | HIS | S | 84 | 28.599 | 43.039 | 26.238 | 1.00 | 0.00 |
| ATOM | 2101 | O | HIS | S | 84 | 29.805 | 42.808 | 26.324 | 1.00 | 0.00 |
| ATOM | 2102 | CB | HIS | S | 84 | 27.157 | 45.056 | 26.812 | 1.00 | 0.00 |
| ATOM | 2103 | CG | HIS | S | 84 | 27.981 | 45.511 | 27.993 | 1.00 | 0.00 |
| ATOM | 2104 | ND1 | HIS | S | 84 | 28.254 | 46.804 | 28.252 | 1.00 | 0.00 |
| ATOM | 2105 | CD2 | HIS | S | 84 | 28.581 | 44.720 | 28.978 | 1.00 | 0.00 |
| ATOM | 2106 | CE1 | HIS | S | 84 | 29.023 | 46.843 | 29.386 | 1.00 | 0.00 |
| ATOM | 2107 | NE2 | HIS | S | 84 | 29.224 | 45.554 | 29.827 | 1.00 | 0.00 |
| ATOM | 2108 | H | HIS | S | 84 | 27.806 | 44.762 | 23.671 | 1.00 | 0.00 |
| ATOM | 2109 | HD1 | HIS | S | 84 | 27.928 | 47.608 | 27.776 | 1.00 | 0.00 |
| ATOM | 2110 | N | GLY | S | 85 | 27.700 | 42.139 | 26.616 | 1.00 | 0.00 |
| ATOM | 2111 | CA | GLY | S | 85 | 28.221 | 40.945 | 27.251 | 1.00 | 0.00 |
| ATOM | 2112 | C | GLY | S | 85 | 28.107 | 41.001 | 28.758 | 1.00 | 0.00 |
| ATOM | 2113 | O | GLY | S | 85 | 27.018 | 40.967 | 29.323 | 1.00 | 0.00 |
| ATOM | 2114 | H | GLY | S | 85 | 26.723 | 42.299 | 26.492 | 1.00 | 0.00 |
| ATOM | 2115 | N | LYS | S | 86 | 29.288 | 40.990 | 29.407 | 1.00 | 0.00 |
| ATOM | 2116 | CA | LYS | S | 86 | 29.195 | 40.412 | 30.753 | 1.00 | 0.00 |
| ATOM | 2117 | C | LYS | S | 86 | 29.446 | 41.218 | 32.028 | 1.00 | 0.00 |
| ATOM | 2118 | O | LYS | S | 86 | 29.080 | 40.709 | 33.079 | 1.00 | 0.00 |
| ATOM | 2119 | CB | LYS | S | 86 | 29.919 | 39.049 | 30.833 | 1.00 | 0.00 |
| ATOM | 2120 | CG | LYS | S | 86 | 29.703 | 38.162 | 29.596 | 1.00 | 0.00 |
| ATOM | 2121 | CD | LYS | S | 86 | 30.014 | 36.667 | 29.739 | 1.00 | 0.00 |
| ATOM | 2122 | CE | LYS | S | 86 | 28.920 | 35.903 | 30.493 | 1.00 | 0.00 |
| ATOM | 2123 | NZ | LYS | S | 86 | 29.117 | 34.452 | 30.347 | 1.00 | 0.00 |
| ATOM | 2124 | H | LYS | S | 86 | 30.126 | 41.167 | 28.888 | 1.00 | 0.00 |
| ATOM | 2125 | 1HZ | LYS | S | 86 | 30.014 | 34.140 | 30.767 | 1.00 | 0.00 |
| ATOM | 2126 | 2HZ | LYS | S | 86 | 28.338 | 33.952 | 30.812 | 1.00 | 0.00 |
| ATOM | 2127 | 3HZ | LYS | S | 86 | 29.106 | 34.182 | 29.347 | 1.00 | 0.00 |
| ATOM | 2128 | N | LYS | S | 87 | 30.078 | 42.417 | 31.917 | 1.00 | 0.00 |
| ATOM | 2129 | CA | LYS | S | 87 | 30.596 | 43.210 | 33.060 | 1.00 | 0.00 |
| ATOM | 2130 | C | LYS | S | 87 | 30.162 | 42.886 | 34.500 | 1.00 | 0.00 |
| ATOM | 2131 | O | LYS | S | 87 | 29.480 | 43.661 | 35.172 | 1.00 | 0.00 |
| ATOM | 2132 | CB | LYS | S | 87 | 30.403 | 44.719 | 32.780 | 1.00 | 0.00 |
| ATOM | 2133 | CG | LYS | S | 87 | 31.159 | 45.733 | 33.672 | 1.00 | 0.00 |
| ATOM | 2134 | CD | LYS | S | 87 | 30.624 | 47.169 | 33.516 | 1.00 | 0.00 |
| ATOM | 2135 | CE | LYS | S | 87 | 31.132 | 48.194 | 34.550 | 1.00 | 0.00 |
| ATOM | 2136 | NZ | LYS | S | 87 | 32.417 | 48.801 | 34.171 | 1.00 | 0.00 |
| ATOM | 2137 | H | LYS | S | 87 | 30.234 | 42.768 | 30.995 | 1.00 | 0.00 |
| ATOM | 2138 | 1HZ | LYS | S | 87 | 33.097 | 48.092 | 33.826 | 1.00 | 0.00 |
| ATOM | 2139 | 2HZ | LYS | S | 87 | 32.295 | 49.571 | 33.489 | 1.00 | 0.00 |
| ATOM | 2140 | 3HZ | LYS | S | 87 | 32.918 | 49.219 | 34.984 | 1.00 | 0.00 |
| ATOM | 2141 | N | ILE | S | 88 | 30.636 | 41.743 | 34.993 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2142 | CA | ILE | S | 88 | 30.224 | 41.419 | 36.352 | 1.00 | 0.00 |
| ATOM | 2143 | C | ILE | S | 88 | 31.419 | 41.186 | 37.247 | 1.00 | 0.00 |
| ATOM | 2144 | O | ILE | S | 88 | 32.209 | 40.276 | 37.032 | 1.00 | 0.00 |
| ATOM | 2145 | CB | ILE | S | 88 | 29.196 | 40.266 | 36.375 | 1.00 | 0.00 |
| ATOM | 2146 | CG1 | ILE | S | 88 | 28.674 | 40.002 | 37.792 | 1.00 | 0.00 |
| ATOM | 2147 | CG2 | ILE | S | 88 | 29.744 | 38.980 | 35.736 | 1.00 | 0.00 |
| ATOM | 2148 | CD1 | ILE | S | 88 | 27.537 | 38.979 | 37.835 | 1.00 | 0.00 |
| ATOM | 2149 | H | ILE | S | 88 | 31.277 | 41.176 | 34.475 | 1.00 | 0.00 |
| ATOM | 2150 | N | ASN | S | 89 | 31.525 | 42.101 | 38.234 | 1.00 | 0.00 |
| ATOM | 2151 | CA | ASN | S | 89 | 32.584 | 42.010 | 39.251 | 1.00 | 0.00 |
| ATOM | 2152 | C | ASN | S | 89 | 33.952 | 41.606 | 38.725 | 1.00 | 0.00 |
| ATOM | 2153 | O | ASN | S | 89 | 34.384 | 40.457 | 38.825 | 1.00 | 0.00 |
| ATOM | 2154 | CB | ASN | S | 89 | 32.139 | 41.086 | 40.384 | 1.00 | 0.00 |
| ATOM | 2155 | CG | ASN | S | 89 | 33.057 | 41.242 | 41.577 | 1.00 | 0.00 |
| ATOM | 2156 | OD1 | ASN | S | 89 | 32.886 | 42.117 | 42.412 | 1.00 | 0.00 |
| ATOM | 2157 | ND2 | ASN | S | 89 | 33.980 | 40.283 | 41.684 | 1.00 | 0.00 |
| ATOM | 2158 | H | ASN | S | 89 | 30.794 | 42.764 | 38.394 | 1.00 | 0.00 |
| ATOM | 2159 | 1HD2 | ASN | S | 89 | 34.456 | 40.102 | 42.547 | 1.00 | 0.00 |
| ATOM | 2160 | 2HD2 | ASN | S | 89 | 34.199 | 39.759 | 40.856 | 1.00 | 0.00 |
| ATOM | 2161 | N | GLY | S | 90 | 34.576 | 42.595 | 38.078 | 1.00 | 0.00 |
| ATOM | 2162 | CA | GLY | S | 90 | 35.815 | 42.291 | 37.371 | 1.00 | 0.00 |
| ATOM | 2163 | C | GLY | S | 90 | 35.621 | 41.634 | 36.014 | 1.00 | 0.00 |
| ATOM | 2164 | O | GLY | S | 90 | 36.040 | 42.139 | 34.975 | 1.00 | 0.00 |
| ATOM | 2165 | H | GLY | S | 90 | 34.200 | 43.515 | 38.133 | 1.00 | 0.00 |
| ATOM | 2166 | N | THR | S | 91 | 34.994 | 40.448 | 36.028 | 1.00 | 0.00 |
| ATOM | 2167 | CA | THR | S | 91 | 35.062 | 39.721 | 34.762 | 1.00 | 0.00 |
| ATOM | 2168 | C | THR | S | 91 | 34.222 | 40.284 | 33.626 | 1.00 | 0.00 |
| ATOM | 2169 | O | THR | S | 91 | 33.133 | 40.834 | 33.774 | 1.00 | 0.00 |
| ATOM | 2170 | CB | THR | S | 91 | 34.878 | 38.205 | 34.938 | 1.00 | 0.00 |
| ATOM | 2171 | OG1 | THR | S | 91 | 35.310 | 37.512 | 33.754 | 1.00 | 0.00 |
| ATOM | 2172 | CG2 | THR | S | 91 | 33.455 | 37.794 | 35.323 | 1.00 | 0.00 |
| ATOM | 2173 | H | THR | S | 91 | 34.509 | 40.120 | 36.842 | 1.00 | 0.00 |
| ATOM | 2174 | HG1 | THR | S | 91 | 35.558 | 36.650 | 34.082 | 1.00 | 0.00 |
| ATOM | 2175 | N | TRP | S | 92 | 34.830 | 40.154 | 32.448 | 1.00 | 0.00 |
| ATOM | 2176 | CA | TRP | S | 92 | 34.259 | 40.801 | 31.285 | 1.00 | 0.00 |
| ATOM | 2177 | C | TRP | S | 92 | 34.705 | 40.058 | 30.048 | 1.00 | 0.00 |
| ATOM | 2178 | O | TRP | S | 92 | 35.885 | 39.888 | 29.773 | 1.00 | 0.00 |
| ATOM | 2179 | CB | TRP | S | 92 | 34.691 | 42.272 | 31.269 | 1.00 | 0.00 |
| ATOM | 2180 | CG | TRP | S | 92 | 33.779 | 43.151 | 30.443 | 1.00 | 0.00 |
| ATOM | 2181 | CD1 | TRP | S | 92 | 32.956 | 42.784 | 29.365 | 1.00 | 0.00 |
| ATOM | 2182 | CD2 | TRP | S | 92 | 33.603 | 44.577 | 30.582 | 1.00 | 0.00 |
| ATOM | 2183 | NE1 | TRP | S | 92 | 32.311 | 43.859 | 28.844 | 1.00 | 0.00 |
| ATOM | 2184 | CE2 | TRP | S | 92 | 32.686 | 44.990 | 29.559 | 1.00 | 0.00 |
| ATOM | 2185 | CE3 | TRP | S | 92 | 34.137 | 45.530 | 31.475 | 1.00 | 0.00 |
| ATOM | 2186 | CZ2 | TRP | S | 92 | 32.336 | 46.352 | 29.441 | 1.00 | 0.00 |
| ATOM | 2187 | CZ3 | TRP | S | 92 | 33.773 | 46.889 | 31.346 | 1.00 | 0.00 |
| ATOM | 2188 | CH2 | TRP | S | 92 | 32.881 | 47.299 | 30.332 | 1.00 | 0.00 |
| ATOM | 2189 | H | TRP | S | 92 | 35.709 | 39.677 | 32.374 | 1.00 | 0.00 |
| ATOM | 2190 | HE1 | TRP | S | 92 | 31.630 | 43.837 | 28.131 | 1.00 | 0.00 |
| ATOM | 2191 | N | ASN | S | 93 | 33.685 | 39.608 | 29.315 | 1.00 | 0.00 |
| ATOM | 2192 | CA | ASN | S | 93 | 33.914 | 39.131 | 27.955 | 1.00 | 0.00 |
| ATOM | 2193 | C | ASN | S | 93 | 32.703 | 39.552 | 27.144 | 1.00 | 0.00 |
| ATOM | 2194 | O | ASN | S | 93 | 31.717 | 39.996 | 27.737 | 1.00 | 0.00 |
| ATOM | 2195 | CB | ASN | S | 93 | 34.249 | 37.625 | 27.890 | 1.00 | 0.00 |
| ATOM | 2196 | CG | ASN | S | 93 | 35.160 | 37.405 | 26.690 | 1.00 | 0.00 |
| ATOM | 2197 | OD1 | ASN | S | 93 | 35.373 | 38.318 | 25.910 | 1.00 | 0.00 |
| ATOM | 2198 | ND2 | ASN | S | 93 | 35.666 | 36.176 | 26.526 | 1.00 | 0.00 |
| ATOM | 2199 | H | ASN | S | 93 | 32.758 | 39.840 | 29.600 | 1.00 | 0.00 |
| ATOM | 2200 | 1HD2 | ASN | S | 93 | 36.149 | 35.985 | 25.664 | 1.00 | 0.00 |
| ATOM | 2201 | 2HD2 | ASN | S | 93 | 35.624 | 35.460 | 27.220 | 1.00 | 0.00 |
| ATOM | 2202 | N | GLY | S | 94 | 32.808 | 39.464 | 25.814 | 1.00 | 0.00 |
| ATOM | 2203 | CA | GLY | S | 94 | 31.973 | 40.347 | 25.005 | 1.00 | 0.00 |
| ATOM | 2204 | C | GLY | S | 94 | 32.818 | 41.583 | 24.815 | 1.00 | 0.00 |
| ATOM | 2205 | O | GLY | S | 94 | 34.015 | 41.449 | 24.583 | 1.00 | 0.00 |
| ATOM | 2206 | H | GLY | S | 94 | 33.653 | 39.082 | 25.431 | 1.00 | 0.00 |
| ATOM | 2207 | N | MET | S | 95 | 32.195 | 42.752 | 25.042 | 1.00 | 0.00 |
| ATOM | 2208 | CA | MET | S | 95 | 32.857 | 44.066 | 24.990 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2209 | C | MET | S | 95 | 34.317 | 44.143 | 25.442 | 1.00 | 0.00 |
| ATOM | 2210 | O | MET | S | 95 | 35.210 | 43.765 | 24.688 | 1.00 | 0.00 |
| ATOM | 2211 | CB | MET | S | 95 | 31.980 | 45.121 | 25.660 | 1.00 | 0.00 |
| ATOM | 2212 | CG | MET | S | 95 | 32.230 | 46.508 | 25.084 | 1.00 | 0.00 |
| ATOM | 2213 | SD | MET | S | 95 | 31.331 | 47.785 | 25.959 | 1.00 | 0.00 |
| ATOM | 2214 | CE | MET | S | 95 | 31.657 | 49.096 | 24.773 | 1.00 | 0.00 |
| ATOM | 2215 | H | MET | S | 95 | 31.197 | 42.708 | 25.076 | 1.00 | 0.00 |
| ATOM | 2216 | N | ILE | S | 96 | 34.598 | 44.584 | 26.689 | 1.00 | 0.00 |
| ATOM | 2217 | CA | ILE | S | 96 | 36.025 | 44.470 | 27.019 | 1.00 | 0.00 |
| ATOM | 2218 | C | ILE | S | 96 | 36.445 | 43.172 | 27.691 | 1.00 | 0.00 |
| ATOM | 2219 | O | ILE | S | 96 | 36.810 | 43.005 | 28.858 | 1.00 | 0.00 |
| ATOM | 2220 | CB | ILE | S | 96 | 36.673 | 45.750 | 27.577 | 1.00 | 0.00 |
| ATOM | 2221 | CG1 | ILE | S | 96 | 36.366 | 46.085 | 29.029 | 1.00 | 0.00 |
| ATOM | 2222 | CG2 | ILE | S | 96 | 36.308 | 46.914 | 26.651 | 1.00 | 0.00 |
| ATOM | 2223 | CD1 | ILE | S | 96 | 37.564 | 45.875 | 29.962 | 1.00 | 0.00 |
| ATOM | 2224 | H | ILE | S | 96 | 33.920 | 44.894 | 27.355 | 1.00 | 0.00 |
| ATOM | 2225 | N | GLY | S | 97 | 36.352 | 42.217 | 26.761 | 1.00 | 0.00 |
| ATOM | 2226 | CA | GLY | S | 97 | 36.918 | 40.893 | 26.891 | 1.00 | 0.00 |
| ATOM | 2227 | C | GLY | S | 97 | 37.509 | 40.450 | 25.566 | 1.00 | 0.00 |
| ATOM | 2228 | O | GLY | S | 97 | 38.583 | 39.866 | 25.538 | 1.00 | 0.00 |
| ATOM | 2229 | H | GLY | S | 97 | 35.918 | 42.463 | 25.896 | 1.00 | 0.00 |
| ATOM | 2230 | N | GLU | S | 98 | 36.781 | 40.754 | 24.476 | 1.00 | 0.00 |
| ATOM | 2231 | CA | GLU | S | 98 | 37.325 | 40.390 | 23.159 | 1.00 | 0.00 |
| ATOM | 2232 | C | GLU | S | 98 | 37.934 | 41.541 | 22.379 | 1.00 | 0.00 |
| ATOM | 2233 | O | GLU | S | 98 | 38.792 | 41.391 | 21.504 | 1.00 | 0.00 |
| ATOM | 2234 | CB | GLU | S | 98 | 36.308 | 39.619 | 22.312 | 1.00 | 0.00 |
| ATOM | 2235 | CG | GLU | S | 98 | 35.821 | 38.279 | 22.895 | 1.00 | 0.00 |
| ATOM | 2236 | CD | GLU | S | 98 | 36.921 | 37.228 | 23.056 | 1.00 | 0.00 |
| ATOM | 2237 | OE1 | GLU | S | 98 | 37.990 | 37.514 | 23.571 | 1.00 | 0.00 |
| ATOM | 2238 | OE2 | GLU | S | 98 | 36.721 | 36.084 | 22.679 | 1.00 | 0.00 |
| ATOM | 2239 | H | GLU | S | 98 | 35.914 | 41.243 | 24.547 | 1.00 | 0.00 |
| ATOM | 2240 | N | VAL | S | 99 | 37.528 | 42.743 | 22.827 | 1.00 | 0.00 |
| ATOM | 2241 | CA | VAL | S | 99 | 38.400 | 43.910 | 22.694 | 1.00 | 0.00 |
| ATOM | 2242 | C | VAL | S | 99 | 39.758 | 43.639 | 23.313 | 1.00 | 0.00 |
| ATOM | 2243 | O | VAL | S | 99 | 40.801 | 43.995 | 22.777 | 1.00 | 0.00 |
| ATOM | 2244 | CB | VAL | S | 99 | 37.751 | 45.135 | 23.362 | 1.00 | 0.00 |
| ATOM | 2245 | CG1 | VAL | S | 99 | 38.635 | 46.376 | 23.438 | 1.00 | 0.00 |
| ATOM | 2246 | CG2 | VAL | S | 99 | 36.476 | 45.504 | 22.634 | 1.00 | 0.00 |
| ATOM | 2247 | H | VAL | S | 99 | 36.666 | 42.786 | 23.327 | 1.00 | 0.00 |
| ATOM | 2248 | N | VAL | S | 100 | 39.682 | 42.979 | 24.483 | 1.00 | 0.00 |
| ATOM | 2249 | CA | VAL | S | 100 | 40.964 | 42.612 | 25.068 | 1.00 | 0.00 |
| ATOM | 2250 | C | VAL | S | 100 | 41.689 | 41.581 | 24.221 | 1.00 | 0.00 |
| ATOM | 2251 | O | VAL | S | 100 | 42.804 | 41.792 | 23.745 | 1.00 | 0.00 |
| ATOM | 2252 | CB | VAL | S | 100 | 40.770 | 42.146 | 26.521 | 1.00 | 0.00 |
| ATOM | 2253 | CG1 | VAL | S | 100 | 42.077 | 41.704 | 27.183 | 1.00 | 0.00 |
| ATOM | 2254 | CG2 | VAL | S | 100 | 40.078 | 43.233 | 27.345 | 1.00 | 0.00 |
| ATOM | 2255 | H | VAL | S | 100 | 38.843 | 42.485 | 24.690 | 1.00 | 0.00 |
| ATOM | 2256 | N | MET | S | 101 | 41.014 | 40.439 | 24.051 | 1.00 | 0.00 |
| ATOM | 2257 | CA | MET | S | 101 | 41.773 | 39.285 | 23.587 | 1.00 | 0.00 |
| ATOM | 2258 | C | MET | S | 101 | 41.785 | 38.998 | 22.087 | 1.00 | 0.00 |
| ATOM | 2259 | O | MET | S | 101 | 42.147 | 37.893 | 21.678 | 1.00 | 0.00 |
| ATOM | 2260 | CB | MET | S | 101 | 41.340 | 38.052 | 24.385 | 1.00 | 0.00 |
| ATOM | 2261 | CG | MET | S | 101 | 41.444 | 38.210 | 25.902 | 1.00 | 0.00 |
| ATOM | 2262 | SD | MET | S | 101 | 40.618 | 36.895 | 26.816 | 1.00 | 0.00 |
| ATOM | 2263 | CE | MET | S | 101 | 40.945 | 37.516 | 28.473 | 1.00 | 0.00 |
| ATOM | 2264 | H | MET | S | 101 | 40.058 | 40.317 | 24.318 | 1.00 | 0.00 |
| ATOM | 2265 | N | LYS | S | 102 | 41.411 | 40.018 | 21.287 | 1.00 | 0.00 |
| ATOM | 2266 | CA | LYS | S | 102 | 41.495 | 40.002 | 19.816 | 1.00 | 0.00 |
| ATOM | 2267 | C | LYS | S | 102 | 40.327 | 39.461 | 18.982 | 1.00 | 0.00 |
| ATOM | 2268 | O | LYS | S | 102 | 40.429 | 39.462 | 17.757 | 1.00 | 0.00 |
| ATOM | 2269 | CB | LYS | S | 102 | 42.803 | 39.405 | 19.243 | 1.00 | 0.00 |
| ATOM | 2270 | CG | LYS | S | 102 | 44.067 | 40.274 | 19.133 | 1.00 | 0.00 |
| ATOM | 2271 | CD | LYS | S | 102 | 44.668 | 40.782 | 20.445 | 1.00 | 0.00 |
| ATOM | 2272 | CE | LYS | S | 102 | 46.113 | 41.295 | 20.313 | 1.00 | 0.00 |
| ATOM | 2273 | NZ | LYS | S | 102 | 46.232 | 42.437 | 19.397 | 1.00 | 0.00 |
| ATOM | 2274 | H | LYS | S | 102 | 40.993 | 40.810 | 21.737 | 1.00 | 0.00 |
| ATOM | 2275 | 1HZ | LYS | S | 102 | 46.207 | 42.188 | 18.393 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2276 | 2HZ | LYS | S | 102 | 45.462 | 43.106 | 19.574 | 1.00 | 0.00 |
| ATOM | 2277 | 3HZ | LYS | S | 102 | 47.111 | 42.974 | 19.553 | 1.00 | 0.00 |
| ATOM | 2278 | N | ARG | S | 103 | 39.217 | 39.008 | 19.622 | 1.00 | 0.00 |
| ATOM | 2279 | CA | ARG | S | 103 | 38.109 | 38.662 | 18.695 | 1.00 | 0.00 |
| ATOM | 2280 | C | ARG | S | 103 | 37.309 | 39.852 | 18.189 | 1.00 | 0.00 |
| ATOM | 2281 | O | ARG | S | 103 | 36.414 | 39.791 | 17.342 | 1.00 | 0.00 |
| ATOM | 2282 | CB | ARG | S | 103 | 37.114 | 37.664 | 19.285 | 1.00 | 0.00 |
| ATOM | 2283 | CG | ARG | S | 103 | 37.184 | 36.247 | 18.707 | 1.00 | 0.00 |
| ATOM | 2284 | CD | ARG | S | 103 | 38.468 | 35.519 | 19.093 | 1.00 | 0.00 |
| ATOM | 2285 | NE | ARG | S | 103 | 38.659 | 35.620 | 20.534 | 1.00 | 0.00 |
| ATOM | 2286 | CZ | ARG | S | 103 | 39.883 | 35.744 | 21.072 | 1.00 | 0.00 |
| ATOM | 2287 | NH1 | ARG | S | 103 | 39.985 | 36.000 | 22.363 | 1.00 | 0.00 |
| ATOM | 2288 | NH2 | ARG | S | 103 | 40.978 | 35.601 | 20.331 | 1.00 | 0.00 |
| ATOM | 2289 | H | ARG | S | 103 | 39.076 | 39.256 | 20.583 | 1.00 | 0.00 |
| ATOM | 2290 | HE | ARG | S | 103 | 37.864 | 35.691 | 21.140 | 1.00 | 0.00 |
| ATOM | 2291 | 1HH1 | ARG | S | 103 | 40.875 | 36.036 | 22.810 | 1.00 | 0.00 |
| ATOM | 2292 | 2HH1 | ARG | S | 103 | 39.160 | 36.205 | 22.904 | 1.00 | 0.00 |
| ATOM | 2293 | 1HH2 | ARG | S | 103 | 41.880 | 35.743 | 20.736 | 1.00 | 0.00 |
| ATOM | 2294 | 2HH2 | ARG | S | 103 | 40.910 | 35.341 | 19.371 | 1.00 | 0.00 |
| ATOM | 2295 | N | ALA | S | 104 | 37.640 | 40.956 | 18.844 | 1.00 | 0.00 |
| ATOM | 2296 | CA | ALA | S | 104 | 37.459 | 42.257 | 18.256 | 1.00 | 0.00 |
| ATOM | 2297 | C | ALA | S | 104 | 38.844 | 42.870 | 18.268 | 1.00 | 0.00 |
| ATOM | 2298 | O | ALA | S | 104 | 39.852 | 42.217 | 18.550 | 1.00 | 0.00 |
| ATOM | 2299 | CB | ALA | S | 104 | 36.519 | 43.064 | 19.150 | 1.00 | 0.00 |
| ATOM | 2300 | H | ALA | S | 104 | 38.285 | 40.937 | 19.600 | 1.00 | 0.00 |
| ATOM | 2301 | N | TYR | S | 105 | 38.891 | 44.173 | 18.034 | 1.00 | 0.00 |
| ATOM | 2302 | CA | TYR | S | 105 | 40.010 | 44.884 | 18.654 | 1.00 | 0.00 |
| ATOM | 2303 | C | TYR | S | 105 | 39.500 | 45.917 | 19.629 | 1.00 | 0.00 |
| ATOM | 2304 | O | TYR | S | 105 | 40.045 | 46.169 | 20.707 | 1.00 | 0.00 |
| ATOM | 2305 | CB | TYR | S | 105 | 40.911 | 45.557 | 17.613 | 1.00 | 0.00 |
| ATOM | 2306 | CG | TYR | S | 105 | 42.225 | 44.824 | 17.438 | 1.00 | 0.00 |
| ATOM | 2307 | CD1 | TYR | S | 105 | 43.430 | 45.532 | 17.625 | 1.00 | 0.00 |
| ATOM | 2308 | CD2 | TYR | S | 105 | 42.219 | 43.463 | 17.075 | 1.00 | 0.00 |
| ATOM | 2309 | CE1 | TYR | S | 105 | 44.655 | 44.869 | 17.435 | 1.00 | 0.00 |
| ATOM | 2310 | CE2 | TYR | S | 105 | 43.438 | 42.800 | 16.880 | 1.00 | 0.00 |
| ATOM | 2311 | CZ | TYR | S | 105 | 44.640 | 43.509 | 17.065 | 1.00 | 0.00 |
| ATOM | 2312 | OH | TYR | S | 105 | 45.834 | 42.830 | 16.873 | 1.00 | 0.00 |
| ATOM | 2313 | H | TYR | S | 105 | 38.081 | 44.613 | 17.642 | 1.00 | 0.00 |
| ATOM | 2314 | HH | TYR | S | 105 | 45.859 | 42.729 | 15.910 | 1.00 | 0.00 |
| ATOM | 2315 | N | MET | S | 106 | 38.409 | 46.532 | 19.164 | 1.00 | 0.00 |
| ATOM | 2316 | CA | MET | S | 106 | 37.808 | 47.670 | 19.841 | 1.00 | 0.00 |
| ATOM | 2317 | C | MET | S | 106 | 36.321 | 47.357 | 19.917 | 1.00 | 0.00 |
| ATOM | 2318 | O | MET | S | 106 | 35.887 | 46.281 | 19.498 | 1.00 | 0.00 |
| ATOM | 2319 | CB | MET | S | 106 | 38.217 | 48.908 | 19.022 | 1.00 | 0.00 |
| ATOM | 2320 | CG | MET | S | 106 | 37.806 | 50.308 | 19.479 | 1.00 | 0.00 |
| ATOM | 2321 | SD | MET | S | 106 | 36.146 | 50.688 | 18.913 | 1.00 | 0.00 |
| ATOM | 2322 | CE | MET | S | 106 | 36.071 | 52.429 | 19.341 | 1.00 | 0.00 |
| ATOM | 2323 | H | MET | S | 106 | 37.994 | 46.188 | 18.325 | 1.00 | 0.00 |
| ATOM | 2324 | N | ALA | S | 107 | 35.536 | 48.288 | 20.452 | 1.00 | 0.00 |
| ATOM | 2325 | CA | ALA | S | 107 | 34.101 | 48.085 | 20.406 | 1.00 | 0.00 |
| ATOM | 2326 | C | ALA | S | 107 | 33.394 | 49.358 | 20.028 | 1.00 | 0.00 |
| ATOM | 2327 | O | ALA | S | 107 | 32.969 | 50.113 | 20.897 | 1.00 | 0.00 |
| ATOM | 2328 | CB | ALA | S | 107 | 33.576 | 47.623 | 21.763 | 1.00 | 0.00 |
| ATOM | 2329 | H | ALA | S | 107 | 35.914 | 49.133 | 20.815 | 1.00 | 0.00 |
| ATOM | 2330 | N | VAL | S | 108 | 33.276 | 49.603 | 18.702 | 1.00 | 0.00 |
| ATOM | 2331 | CA | VAL | S | 108 | 32.669 | 50.875 | 18.291 | 1.00 | 0.00 |
| ATOM | 2332 | C | VAL | S | 108 | 31.159 | 50.983 | 18.440 | 1.00 | 0.00 |
| ATOM | 2333 | O | VAL | S | 108 | 30.371 | 50.829 | 17.513 | 1.00 | 0.00 |
| ATOM | 2334 | CB | VAL | S | 108 | 33.062 | 51.375 | 16.888 | 1.00 | 0.00 |
| ATOM | 2335 | CG1 | VAL | S | 108 | 33.193 | 52.899 | 16.951 | 1.00 | 0.00 |
| ATOM | 2336 | CG2 | VAL | S | 108 | 34.302 | 50.750 | 16.255 | 1.00 | 0.00 |
| ATOM | 2337 | H | VAL | S | 108 | 33.465 | 48.889 | 18.029 | 1.00 | 0.00 |
| ATOM | 2338 | N | GLY | S | 109 | 30.836 | 51.336 | 19.679 | 1.00 | 0.00 |
| ATOM | 2339 | CA | GLY | S | 109 | 29.671 | 52.088 | 20.110 | 1.00 | 0.00 |
| ATOM | 2340 | C | GLY | S | 109 | 30.294 | 53.008 | 21.134 | 1.00 | 0.00 |
| ATOM | 2341 | O | GLY | S | 109 | 30.534 | 52.655 | 22.288 | 1.00 | 0.00 |
| ATOM | 2342 | H | GLY | S | 109 | 31.519 | 51.179 | 20.387 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2343 | N | SER | S | 110 | 30.726 | 54.175 | 20.618 | 1.00 | 0.00 |
| ATOM | 2344 | CA | SER | S | 110 | 31.449 | 55.193 | 21.402 | 1.00 | 0.00 |
| ATOM | 2345 | C | SER | S | 110 | 32.482 | 54.744 | 22.463 | 1.00 | 0.00 |
| ATOM | 2346 | O | SER | S | 110 | 32.328 | 55.013 | 23.657 | 1.00 | 0.00 |
| ATOM | 2347 | CB | SER | S | 110 | 30.399 | 56.169 | 21.957 | 1.00 | 0.00 |
| ATOM | 2348 | OG | SER | S | 110 | 29.093 | 55.557 | 22.060 | 1.00 | 0.00 |
| ATOM | 2349 | H | SER | S | 110 | 30.367 | 54.350 | 19.703 | 1.00 | 0.00 |
| ATOM | 2350 | HG | SER | S | 110 | 28.490 | 56.303 | 22.153 | 1.00 | 0.00 |
| ATOM | 2351 | N | LEU | S | 111 | 33.514 | 53.991 | 22.012 | 1.00 | 0.00 |
| ATOM | 2352 | CA | LEU | S | 111 | 34.325 | 53.379 | 23.069 | 1.00 | 0.00 |
| ATOM | 2353 | C | LEU | S | 111 | 35.268 | 54.280 | 23.845 | 1.00 | 0.00 |
| ATOM | 2354 | O | LEU | S | 111 | 36.461 | 54.438 | 23.592 | 1.00 | 0.00 |
| ATOM | 2355 | CB | LEU | S | 111 | 35.065 | 52.117 | 22.636 | 1.00 | 0.00 |
| ATOM | 2356 | CG | LEU | S | 111 | 34.807 | 50.912 | 23.545 | 1.00 | 0.00 |
| ATOM | 2357 | CD1 | LEU | S | 111 | 35.848 | 49.828 | 23.331 | 1.00 | 0.00 |
| ATOM | 2358 | CD2 | LEU | S | 111 | 34.738 | 51.251 | 25.025 | 1.00 | 0.00 |
| ATOM | 2359 | H | LEU | S | 111 | 33.819 | 54.048 | 21.065 | 1.00 | 0.00 |
| ATOM | 2360 | N | THR | S | 112 | 34.626 | 54.832 | 24.870 | 1.00 | 0.00 |
| ATOM | 2361 | CA | THR | S | 112 | 35.300 | 55.570 | 25.915 | 1.00 | 0.00 |
| ATOM | 2362 | C | THR | S | 112 | 36.276 | 54.654 | 26.637 | 1.00 | 0.00 |
| ATOM | 2363 | O | THR | S | 112 | 35.969 | 53.500 | 26.964 | 1.00 | 0.00 |
| ATOM | 2364 | CB | THR | S | 112 | 34.217 | 56.087 | 26.870 | 1.00 | 0.00 |
| ATOM | 2365 | OG1 | THR | S | 112 | 33.113 | 56.693 | 26.166 | 1.00 | 0.00 |
| ATOM | 2366 | CG2 | THR | S | 112 | 34.769 | 57.059 | 27.906 | 1.00 | 0.00 |
| ATOM | 2367 | H | THR | S | 112 | 33.654 | 54.621 | 24.929 | 1.00 | 0.00 |
| ATOM | 2368 | HG1 | THR | S | 112 | 32.995 | 56.265 | 25.311 | 1.00 | 0.00 |
| ATOM | 2369 | N | ILE | S | 113 | 37.454 | 55.227 | 26.900 | 1.00 | 0.00 |
| ATOM | 2370 | CA | ILE | S | 113 | 38.306 | 54.549 | 27.869 | 1.00 | 0.00 |
| ATOM | 2371 | C | ILE | S | 113 | 37.648 | 54.737 | 29.209 | 1.00 | 0.00 |
| ATOM | 2372 | O | ILE | S | 113 | 37.318 | 55.871 | 29.548 | 1.00 | 0.00 |
| ATOM | 2373 | CB | ILE | S | 113 | 39.718 | 55.145 | 27.943 | 1.00 | 0.00 |
| ATOM | 2374 | CG1 | ILE | S | 113 | 40.132 | 55.962 | 26.716 | 1.00 | 0.00 |
| ATOM | 2375 | CG2 | ILE | S | 113 | 40.695 | 54.003 | 28.219 | 1.00 | 0.00 |
| ATOM | 2376 | CD1 | ILE | S | 113 | 41.513 | 56.606 | 26.853 | 1.00 | 0.00 |
| ATOM | 2377 | H | ILE | S | 113 | 37.599 | 56.180 | 26.630 | 1.00 | 0.00 |
| ATOM | 2378 | N | ASN | S | 114 | 37.418 | 53.635 | 29.893 | 1.00 | 0.00 |
| ATOM | 2379 | CA | ASN | S | 114 | 37.164 | 53.774 | 31.309 | 1.00 | 0.00 |
| ATOM | 2380 | C | ASN | S | 114 | 38.264 | 52.970 | 31.938 | 1.00 | 0.00 |
| ATOM | 2381 | O | ASN | S | 114 | 38.773 | 52.034 | 31.330 | 1.00 | 0.00 |
| ATOM | 2382 | CB | ASN | S | 114 | 35.786 | 53.239 | 31.686 | 1.00 | 0.00 |
| ATOM | 2383 | CG | ASN | S | 114 | 35.586 | 53.427 | 33.174 | 1.00 | 0.00 |
| ATOM | 2384 | OD1 | ASN | S | 114 | 35.954 | 52.594 | 33.999 | 1.00 | 0.00 |
| ATOM | 2385 | ND2 | ASN | S | 114 | 34.980 | 54.567 | 33.508 | 1.00 | 0.00 |
| ATOM | 2386 | H | ASN | S | 114 | 37.746 | 52.766 | 29.545 | 1.00 | 0.00 |
| ATOM | 2387 | 1HD2 | ASN | S | 114 | 34.831 | 54.749 | 34.482 | 1.00 | 0.00 |
| ATOM | 2388 | 2HD2 | ASN | S | 114 | 34.614 | 55.246 | 32.861 | 1.00 | 0.00 |
| ATOM | 2389 | N | GLU | S | 115 | 38.621 | 53.398 | 33.134 | 1.00 | 0.00 |
| ATOM | 2390 | CA | GLU | S | 115 | 39.642 | 52.804 | 33.985 | 1.00 | 0.00 |
| ATOM | 2391 | C | GLU | S | 115 | 39.789 | 51.280 | 33.885 | 1.00 | 0.00 |
| ATOM | 2392 | O | GLU | S | 115 | 40.882 | 50.756 | 33.689 | 1.00 | 0.00 |
| ATOM | 2393 | CB | GLU | S | 115 | 39.424 | 53.334 | 35.413 | 1.00 | 0.00 |
| ATOM | 2394 | CG | GLU | S | 115 | 39.676 | 54.851 | 35.633 | 1.00 | 0.00 |
| ATOM | 2395 | CD | GLU | S | 115 | 38.686 | 55.798 | 34.940 | 1.00 | 0.00 |
| ATOM | 2396 | OE1 | GLU | S | 115 | 39.083 | 56.860 | 34.473 | 1.00 | 0.00 |
| ATOM | 2397 | OE2 | GLU | S | 115 | 37.502 | 55.497 | 34.854 | 1.00 | 0.00 |
| ATOM | 2398 | H | GLU | S | 115 | 38.210 | 54.266 | 33.393 | 1.00 | 0.00 |
| ATOM | 2399 | N | GLU | S | 116 | 38.642 | 50.571 | 33.932 | 1.00 | 0.00 |
| ATOM | 2400 | CA | GLU | S | 116 | 38.696 | 49.111 | 33.733 | 1.00 | 0.00 |
| ATOM | 2401 | C | GLU | S | 116 | 39.407 | 48.667 | 32.458 | 1.00 | 0.00 |
| ATOM | 2402 | O | GLU | S | 116 | 40.285 | 47.811 | 32.422 | 1.00 | 0.00 |
| ATOM | 2403 | CB | GLU | S | 116 | 37.284 | 48.535 | 33.758 | 1.00 | 0.00 |
| ATOM | 2404 | CG | GLU | S | 116 | 36.635 | 48.654 | 35.138 | 1.00 | 0.00 |
| ATOM | 2405 | CD | GLU | S | 116 | 35.162 | 48.298 | 35.078 | 1.00 | 0.00 |
| ATOM | 2406 | OE1 | GLU | S | 116 | 34.739 | 47.518 | 34.234 | 1.00 | 0.00 |
| ATOM | 2407 | OE2 | GLU | S | 116 | 34.401 | 48.821 | 35.876 | 1.00 | 0.00 |
| ATOM | 2408 | H | GLU | S | 116 | 37.804 | 51.106 | 34.034 | 1.00 | 0.00 |
| ATOM | 2409 | N | ARG | S | 117 | 38.996 | 49.363 | 31.403 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2410 | CA | ARG | S | 117 | 39.587 | 49.215 | 30.082 | 1.00 | 0.00 |
| ATOM | 2411 | C | ARG | S | 117 | 41.050 | 49.645 | 30.018 | 1.00 | 0.00 |
| ATOM | 2412 | O | ARG | S | 117 | 41.901 | 48.930 | 29.502 | 1.00 | 0.00 |
| ATOM | 2413 | CB | ARG | S | 117 | 38.705 | 49.986 | 29.087 | 1.00 | 0.00 |
| ATOM | 2414 | CG | ARG | S | 117 | 37.222 | 49.606 | 29.214 | 1.00 | 0.00 |
| ATOM | 2415 | CD | ARG | S | 117 | 36.226 | 50.518 | 28.493 | 1.00 | 0.00 |
| ATOM | 2416 | NE | ARG | S | 117 | 34.939 | 49.839 | 28.298 | 1.00 | 0.00 |
| ATOM | 2417 | CZ | ARG | S | 117 | 33.769 | 50.507 | 28.168 | 1.00 | 0.00 |
| ATOM | 2418 | NH1 | ARG | S | 117 | 33.731 | 51.814 | 28.416 | 1.00 | 0.00 |
| ATOM | 2419 | NH2 | ARG | S | 117 | 32.668 | 49.857 | 27.790 | 1.00 | 0.00 |
| ATOM | 2420 | H | ARG | S | 117 | 38.326 | 50.067 | 31.617 | 1.00 | 0.00 |
| ATOM | 2421 | HE | ARG | S | 117 | 34.980 | 48.877 | 28.002 | 1.00 | 0.00 |
| ATOM | 2422 | 1HH1 | ARG | S | 117 | 32.881 | 52.330 | 28.323 | 1.00 | 0.00 |
| ATOM | 2423 | 2HH1 | ARG | S | 117 | 34.551 | 52.310 | 28.707 | 1.00 | 0.00 |
| ATOM | 2424 | 1HH2 | ARG | S | 117 | 31.805 | 50.330 | 27.578 | 1.00 | 0.00 |
| ATOM | 2425 | 2HH2 | ARG | S | 117 | 32.682 | 48.863 | 27.646 | 1.00 | 0.00 |
| ATOM | 2426 | N | SER | S | 118 | 41.300 | 50.843 | 30.577 | 1.00 | 0.00 |
| ATOM | 2427 | CA | SER | S | 118 | 42.533 | 51.597 | 30.326 | 1.00 | 0.00 |
| ATOM | 2428 | C | SER | S | 118 | 43.838 | 50.858 | 30.061 | 1.00 | 0.00 |
| ATOM | 2429 | O | SER | S | 118 | 44.394 | 50.937 | 28.968 | 1.00 | 0.00 |
| ATOM | 2430 | CB | SER | S | 118 | 42.737 | 52.661 | 31.409 | 1.00 | 0.00 |
| ATOM | 2431 | OG | SER | S | 118 | 41.610 | 53.552 | 31.456 | 1.00 | 0.00 |
| ATOM | 2432 | H | SER | S | 118 | 40.562 | 51.306 | 31.065 | 1.00 | 0.00 |
| ATOM | 2433 | HG | SER | S | 118 | 41.576 | 53.854 | 32.364 | 1.00 | 0.00 |
| ATOM | 2434 | N | GLU | S | 119 | 44.324 | 50.171 | 31.092 | 1.00 | 0.00 |
| ATOM | 2435 | CA | GLU | S | 119 | 45.704 | 49.746 | 30.889 | 1.00 | 0.00 |
| ATOM | 2436 | C | GLU | S | 119 | 45.889 | 48.418 | 30.177 | 1.00 | 0.00 |
| ATOM | 2437 | O | GLU | S | 119 | 46.963 | 48.063 | 29.678 | 1.00 | 0.00 |
| ATOM | 2438 | CB | GLU | S | 119 | 46.517 | 49.940 | 32.175 | 1.00 | 0.00 |
| ATOM | 2439 | CG | GLU | S | 119 | 47.973 | 50.399 | 31.957 | 1.00 | 0.00 |
| ATOM | 2440 | CD | GLU | S | 119 | 48.106 | 51.651 | 31.083 | 1.00 | 0.00 |
| ATOM | 2441 | OE1 | GLU | S | 119 | 49.157 | 51.841 | 30.482 | 1.00 | 0.00 |
| ATOM | 2442 | OE2 | GLU | S | 119 | 47.169 | 52.431 | 30.934 | 1.00 | 0.00 |
| ATOM | 2443 | H | GLU | S | 119 | 43.807 | 49.954 | 31.913 | 1.00 | 0.00 |
| ATOM | 2444 | N | VAL | S | 120 | 44.745 | 47.726 | 30.070 | 1.00 | 0.00 |
| ATOM | 2445 | CA | VAL | S | 120 | 44.774 | 46.734 | 29.010 | 1.00 | 0.00 |
| ATOM | 2446 | C | VAL | S | 120 | 44.346 | 47.368 | 27.695 | 1.00 | 0.00 |
| ATOM | 2447 | O | VAL | S | 120 | 45.151 | 47.733 | 26.837 | 1.00 | 0.00 |
| ATOM | 2448 | CB | VAL | S | 120 | 43.938 | 45.495 | 29.358 | 1.00 | 0.00 |
| ATOM | 2449 | CG1 | VAL | S | 120 | 44.258 | 44.364 | 28.379 | 1.00 | 0.00 |
| ATOM | 2450 | CG2 | VAL | S | 120 | 44.149 | 45.051 | 30.808 | 1.00 | 0.00 |
| ATOM | 2451 | H | VAL | S | 120 | 43.902 | 48.074 | 30.466 | 1.00 | 0.00 |
| ATOM | 2452 | N | VAL | S | 121 | 43.030 | 47.503 | 27.544 | 1.00 | 0.00 |
| ATOM | 2453 | CA | VAL | S | 121 | 42.565 | 48.172 | 26.338 | 1.00 | 0.00 |
| ATOM | 2454 | C | VAL | S | 121 | 42.345 | 49.673 | 26.472 | 1.00 | 0.00 |
| ATOM | 2455 | O | VAL | S | 121 | 41.301 | 50.161 | 26.885 | 1.00 | 0.00 |
| ATOM | 2456 | CB | VAL | S | 121 | 41.345 | 47.428 | 25.798 | 1.00 | 0.00 |
| ATOM | 2457 | CG1 | VAL | S | 121 | 41.817 | 46.086 | 25.256 | 1.00 | 0.00 |
| ATOM | 2458 | CG2 | VAL | S | 121 | 40.247 | 47.216 | 26.845 | 1.00 | 0.00 |
| ATOM | 2459 | H | VAL | S | 121 | 42.455 | 47.370 | 28.351 | 1.00 | 0.00 |
| ATOM | 2460 | N | ASP | S | 122 | 43.393 | 50.434 | 26.088 | 1.00 | 0.00 |
| ATOM | 2461 | CA | ASP | S | 122 | 43.110 | 51.881 | 26.053 | 1.00 | 0.00 |
| ATOM | 2462 | C | ASP | S | 122 | 42.550 | 52.317 | 24.721 | 1.00 | 0.00 |
| ATOM | 2463 | O | ASP | S | 122 | 42.641 | 51.556 | 23.757 | 1.00 | 0.00 |
| ATOM | 2464 | CB | ASP | S | 122 | 44.313 | 52.758 | 26.437 | 1.00 | 0.00 |
| ATOM | 2465 | CG | ASP | S | 122 | 45.453 | 52.640 | 25.447 | 1.00 | 0.00 |
| ATOM | 2466 | OD1 | ASP | S | 122 | 46.487 | 52.116 | 25.807 | 1.00 | 0.00 |
| ATOM | 2467 | OD2 | ASP | S | 122 | 45.336 | 53.064 | 24.308 | 1.00 | 0.00 |
| ATOM | 2468 | H | ASP | S | 122 | 44.282 | 50.069 | 25.796 | 1.00 | 0.00 |
| ATOM | 2469 | N | PHE | S | 123 | 41.993 | 53.547 | 24.697 | 1.00 | 0.00 |
| ATOM | 2470 | CA | PHE | S | 123 | 41.268 | 54.039 | 23.515 | 1.00 | 0.00 |
| ATOM | 2471 | C | PHE | S | 123 | 41.718 | 55.419 | 23.014 | 1.00 | 0.00 |
| ATOM | 2472 | O | PHE | S | 123 | 42.872 | 55.593 | 22.645 | 1.00 | 0.00 |
| ATOM | 2473 | CB | PHE | S | 123 | 39.749 | 53.916 | 23.728 | 1.00 | 0.00 |
| ATOM | 2474 | CG | PHE | S | 123 | 39.375 | 52.484 | 24.036 | 1.00 | 0.00 |
| ATOM | 2475 | CD1 | PHE | S | 123 | 38.868 | 52.169 | 25.313 | 1.00 | 0.00 |
| ATOM | 2476 | CD2 | PHE | S | 123 | 39.571 | 51.482 | 23.061 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2477 | CE1 | PHE | S | 123 | 38.623 | 50.825 | 25.644 | 1.00 | 0.00 |
| ATOM | 2478 | CE2 | PHE | S | 123 | 39.341 | 50.135 | 23.393 | 1.00 | 0.00 |
| ATOM | 2479 | CZ | PHE | S | 123 | 38.899 | 49.821 | 24.695 | 1.00 | 0.00 |
| ATOM | 2480 | H | PHE | S | 123 | 42.230 | 54.146 | 25.458 | 1.00 | 0.00 |
| ATOM | 2481 | N | SER | S | 124 | 40.819 | 56.421 | 22.993 | 1.00 | 0.00 |
| ATOM | 2482 | CA | SER | S | 124 | 41.293 | 57.746 | 22.549 | 1.00 | 0.00 |
| ATOM | 2483 | C | SER | S | 124 | 40.611 | 58.862 | 23.342 | 1.00 | 0.00 |
| ATOM | 2484 | O | SER | S | 124 | 39.888 | 58.536 | 24.280 | 1.00 | 0.00 |
| ATOM | 2485 | CB | SER | S | 124 | 41.114 | 57.915 | 21.029 | 1.00 | 0.00 |
| ATOM | 2486 | OG | SER | S | 124 | 41.090 | 56.631 | 20.365 | 1.00 | 0.00 |
| ATOM | 2487 | H | SER | S | 124 | 39.890 | 56.344 | 23.349 | 1.00 | 0.00 |
| ATOM | 2488 | HG | SER | S | 124 | 40.602 | 56.778 | 19.545 | 1.00 | 0.00 |
| ATOM | 2489 | N | VAL | S | 125 | 40.865 | 60.149 | 22.980 | 1.00 | 0.00 |
| ATOM | 2490 | CA | VAL | S | 125 | 40.213 | 61.303 | 23.627 | 1.00 | 0.00 |
| ATOM | 2491 | C | VAL | S | 125 | 39.596 | 62.344 | 22.658 | 1.00 | 0.00 |
| ATOM | 2492 | O | VAL | S | 125 | 38.381 | 62.563 | 22.654 | 1.00 | 0.00 |
| ATOM | 2493 | CB | VAL | S | 125 | 41.126 | 61.973 | 24.690 | 1.00 | 0.00 |
| ATOM | 2494 | CG1 | VAL | S | 125 | 40.380 | 63.049 | 25.483 | 1.00 | 0.00 |
| ATOM | 2495 | CG2 | VAL | S | 125 | 41.806 | 60.972 | 25.627 | 1.00 | 0.00 |
| ATOM | 2496 | H | VAL | S | 125 | 41.430 | 60.323 | 22.174 | 1.00 | 0.00 |
| ATOM | 2497 | N | PRO | S | 126 | 40.429 | 62.992 | 21.786 | 1.00 | 0.00 |
| ATOM | 2498 | CA | PRO | S | 126 | 39.826 | 63.961 | 20.863 | 1.00 | 0.00 |
| ATOM | 2499 | C | PRO | S | 126 | 39.340 | 63.286 | 19.587 | 1.00 | 0.00 |
| ATOM | 2500 | O | PRO | S | 126 | 39.568 | 63.747 | 18.472 | 1.00 | 0.00 |
| ATOM | 2501 | CB | PRO | S | 126 | 41.003 | 64.906 | 20.620 | 1.00 | 0.00 |
| ATOM | 2502 | CG | PRO | S | 126 | 42.218 | 63.979 | 20.568 | 1.00 | 0.00 |
| ATOM | 2503 | CD | PRO | S | 126 | 41.881 | 62.911 | 21.603 | 1.00 | 0.00 |
| ATOM | 2504 | N | PHE | S | 127 | 38.733 | 62.102 | 19.774 | 1.00 | 0.00 |
| ATOM | 2505 | CA | PHE | S | 127 | 38.023 | 61.532 | 18.633 | 1.00 | 0.00 |
| ATOM | 2506 | C | PHE | S | 127 | 36.675 | 62.227 | 18.570 | 1.00 | 0.00 |
| ATOM | 2507 | O | PHE | S | 127 | 36.625 | 63.439 | 18.399 | 1.00 | 0.00 |
| ATOM | 2508 | CB | PHE | S | 127 | 37.960 | 60.009 | 18.785 | 1.00 | 0.00 |
| ATOM | 2509 | CG | PHE | S | 127 | 39.062 | 59.310 | 18.018 | 1.00 | 0.00 |
| ATOM | 2510 | CD1 | PHE | S | 127 | 38.733 | 58.138 | 17.306 | 1.00 | 0.00 |
| ATOM | 2511 | CD2 | PHE | S | 127 | 40.385 | 59.811 | 18.020 | 1.00 | 0.00 |
| ATOM | 2512 | CE1 | PHE | S | 127 | 39.730 | 57.459 | 16.582 | 1.00 | 0.00 |
| ATOM | 2513 | CE2 | PHE | S | 127 | 41.382 | 59.130 | 17.296 | 1.00 | 0.00 |
| ATOM | 2514 | CZ | PHE | S | 127 | 41.047 | 57.961 | 16.584 | 1.00 | 0.00 |
| ATOM | 2515 | H | PHE | S | 127 | 38.465 | 61.883 | 20.709 | 1.00 | 0.00 |
| ATOM | 2516 | N | ILE | S | 128 | 35.590 | 61.484 | 18.790 | 1.00 | 0.00 |
| ATOM | 2517 | CA | ILE | S | 128 | 34.401 | 62.192 | 19.252 | 1.00 | 0.00 |
| ATOM | 2518 | C | ILE | S | 128 | 34.491 | 62.472 | 20.761 | 1.00 | 0.00 |
| ATOM | 2519 | O | ILE | S | 128 | 35.385 | 61.963 | 21.456 | 1.00 | 0.00 |
| ATOM | 2520 | CB | ILE | S | 128 | 33.185 | 61.375 | 18.772 | 1.00 | 0.00 |
| ATOM | 2521 | CG1 | ILE | S | 128 | 31.825 | 62.065 | 18.829 | 1.00 | 0.00 |
| ATOM | 2522 | CG2 | ILE | S | 128 | 33.147 | 60.019 | 19.468 | 1.00 | 0.00 |
| ATOM | 2523 | CD1 | ILE | S | 128 | 30.728 | 61.230 | 18.175 | 1.00 | 0.00 |
| ATOM | 2524 | H | ILE | S | 128 | 35.585 | 60.492 | 18.738 | 1.00 | 0.00 |
| ATOM | 2525 | N | GLU | S | 129 | 33.558 | 63.333 | 21.232 | 1.00 | 0.00 |
| ATOM | 2526 | CA | GLU | S | 129 | 33.604 | 64.060 | 22.514 | 1.00 | 0.00 |
| ATOM | 2527 | C | GLU | S | 129 | 34.345 | 63.473 | 23.696 | 1.00 | 0.00 |
| ATOM | 2528 | O | GLU | S | 129 | 34.524 | 62.260 | 23.838 | 1.00 | 0.00 |
| ATOM | 2529 | CB | GLU | S | 129 | 32.226 | 64.478 | 23.053 | 1.00 | 0.00 |
| ATOM | 2530 | CG | GLU | S | 129 | 31.044 | 64.524 | 22.087 | 1.00 | 0.00 |
| ATOM | 2531 | CD | GLU | S | 129 | 30.383 | 63.163 | 21.921 | 1.00 | 0.00 |
| ATOM | 2532 | OE1 | GLU | S | 129 | 29.322 | 63.122 | 21.330 | 1.00 | 0.00 |
| ATOM | 2533 | OE2 | GLU | S | 129 | 30.890 | 62.139 | 22.365 | 1.00 | 0.00 |
| ATOM | 2534 | H | GLU | S | 129 | 32.835 | 63.548 | 20.576 | 1.00 | 0.00 |
| ATOM | 2535 | N | THR | S | 130 | 34.739 | 64.433 | 24.551 | 1.00 | 0.00 |
| ATOM | 2536 | CA | THR | S | 130 | 35.421 | 64.072 | 25.787 | 1.00 | 0.00 |
| ATOM | 2537 | C | THR | S | 130 | 34.445 | 63.842 | 26.937 | 1.00 | 0.00 |
| ATOM | 2538 | O | THR | S | 130 | 34.261 | 64.660 | 27.837 | 1.00 | 0.00 |
| ATOM | 2539 | CB | THR | S | 130 | 36.478 | 65.129 | 26.147 | 1.00 | 0.00 |
| ATOM | 2540 | OG1 | THR | S | 130 | 37.234 | 65.529 | 24.991 | 1.00 | 0.00 |
| ATOM | 2541 | CG2 | THR | S | 130 | 37.413 | 64.669 | 27.272 | 1.00 | 0.00 |
| ATOM | 2542 | H | THR | S | 130 | 34.502 | 65.376 | 24.323 | 1.00 | 0.00 |
| ATOM | 2543 | HG1 | THR | S | 130 | 36.621 | 65.961 | 24.401 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2544 | N | GLY | S | 131 | 33.797 | 62.666 | 26.885 | 1.00 | 0.00 |
| ATOM | 2545 | CA | GLY | S | 131 | 32.793 | 62.366 | 27.917 | 1.00 | 0.00 |
| ATOM | 2546 | C | GLY | S | 131 | 33.281 | 62.361 | 29.368 | 1.00 | 0.00 |
| ATOM | 2547 | O | GLY | S | 131 | 33.916 | 61.422 | 29.838 | 1.00 | 0.00 |
| ATOM | 2548 | H | GLY | S | 131 | 34.043 | 62.014 | 26.158 | 1.00 | 0.00 |
| ATOM | 2549 | N | ILE | S | 132 | 32.957 | 63.450 | 30.089 | 1.00 | 0.00 |
| ATOM | 2550 | CA | ILE | S | 132 | 33.245 | 63.382 | 31.522 | 1.00 | 0.00 |
| ATOM | 2551 | C | ILE | S | 132 | 31.955 | 63.250 | 32.341 | 1.00 | 0.00 |
| ATOM | 2552 | O | ILE | S | 132 | 31.114 | 62.430 | 31.963 | 1.00 | 0.00 |
| ATOM | 2553 | CB | ILE | S | 132 | 34.266 | 64.472 | 31.909 | 1.00 | 0.00 |
| ATOM | 2554 | CG1 | ILE | S | 132 | 34.917 | 64.287 | 33.286 | 1.00 | 0.00 |
| ATOM | 2555 | CG2 | ILE | S | 132 | 33.673 | 65.866 | 31.730 | 1.00 | 0.00 |
| ATOM | 2556 | CD1 | ILE | S | 132 | 35.691 | 62.973 | 33.410 | 1.00 | 0.00 |
| ATOM | 2557 | H | ILE | S | 132 | 32.407 | 64.200 | 29.721 | 1.00 | 0.00 |
| ATOM | 2558 | N | SER | S | 133 | 31.760 | 63.986 | 33.443 | 1.00 | 0.00 |
| ATOM | 2559 | CA | SER | S | 133 | 30.681 | 63.559 | 34.308 | 1.00 | 0.00 |
| ATOM | 2560 | C | SER | S | 133 | 29.751 | 64.696 | 34.639 | 1.00 | 0.00 |
| ATOM | 2561 | O | SER | S | 133 | 30.109 | 65.737 | 35.189 | 1.00 | 0.00 |
| ATOM | 2562 | CB | SER | S | 133 | 31.276 | 62.819 | 35.506 | 1.00 | 0.00 |
| ATOM | 2563 | OG | SER | S | 133 | 32.198 | 61.821 | 35.008 | 1.00 | 0.00 |
| ATOM | 2564 | H | SER | S | 133 | 32.233 | 64.857 | 33.559 | 1.00 | 0.00 |
| ATOM | 2565 | HG | SER | S | 133 | 31.923 | 61.661 | 34.099 | 1.00 | 0.00 |
| ATOM | 2566 | N | VAL | S | 134 | 28.518 | 64.455 | 34.206 | 1.00 | 0.00 |
| ATOM | 2567 | CA | VAL | S | 134 | 27.472 | 65.468 | 34.293 | 1.00 | 0.00 |
| ATOM | 2568 | C | VAL | S | 134 | 27.322 | 66.122 | 35.648 | 1.00 | 0.00 |
| ATOM | 2569 | O | VAL | S | 134 | 27.247 | 65.490 | 36.699 | 1.00 | 0.00 |
| ATOM | 2570 | CB | VAL | S | 134 | 26.169 | 64.854 | 33.817 | 1.00 | 0.00 |
| ATOM | 2571 | CG1 | VAL | S | 134 | 26.249 | 64.677 | 32.308 | 1.00 | 0.00 |
| ATOM | 2572 | CG2 | VAL | S | 134 | 25.882 | 63.529 | 34.527 | 1.00 | 0.00 |
| ATOM | 2573 | H | VAL | S | 134 | 28.290 | 63.585 | 33.773 | 1.00 | 0.00 |
| ATOM | 2574 | N | MET | S | 135 | 27.373 | 67.458 | 35.593 | 1.00 | 0.00 |
| ATOM | 2575 | CA | MET | S | 135 | 27.111 | 68.192 | 36.822 | 1.00 | 0.00 |
| ATOM | 2576 | C | MET | S | 135 | 25.606 | 68.346 | 37.063 | 1.00 | 0.00 |
| ATOM | 2577 | O | MET | S | 135 | 25.102 | 68.686 | 38.130 | 1.00 | 0.00 |
| ATOM | 2578 | CB | MET | S | 135 | 27.922 | 69.491 | 36.776 | 1.00 | 0.00 |
| ATOM | 2579 | CG | MET | S | 135 | 27.668 | 70.423 | 37.952 | 1.00 | 0.00 |
| ATOM | 2580 | SD | MET | S | 135 | 28.882 | 71.716 | 38.203 | 1.00 | 0.00 |
| ATOM | 2581 | CE | MET | S | 135 | 29.853 | 70.909 | 39.484 | 1.00 | 0.00 |
| ATOM | 2582 | H | MET | S | 135 | 27.316 | 67.920 | 34.711 | 1.00 | 0.00 |
| ATOM | 2583 | N | VAL | S | 136 | 24.875 | 67.994 | 35.985 | 1.00 | 0.00 |
| ATOM | 2584 | CA | VAL | S | 136 | 23.418 | 68.136 | 35.851 | 1.00 | 0.00 |
| ATOM | 2585 | C | VAL | S | 136 | 22.559 | 67.975 | 37.109 | 1.00 | 0.00 |
| ATOM | 2586 | O | VAL | S | 136 | 22.838 | 67.203 | 38.030 | 1.00 | 0.00 |
| ATOM | 2587 | CB | VAL | S | 136 | 22.946 | 67.276 | 34.651 | 1.00 | 0.00 |
| ATOM | 2588 | CG1 | VAL | S | 136 | 21.437 | 67.256 | 34.377 | 1.00 | 0.00 |
| ATOM | 2589 | CG2 | VAL | S | 136 | 23.662 | 67.761 | 33.388 | 1.00 | 0.00 |
| ATOM | 2590 | H | VAL | S | 136 | 25.365 | 67.731 | 35.154 | 1.00 | 0.00 |
| ATOM | 2591 | N | SER | S | 137 | 21.536 | 68.847 | 37.076 | 1.00 | 0.00 |
| ATOM | 2592 | CA | SER | S | 137 | 20.538 | 69.002 | 38.123 | 1.00 | 0.00 |
| ATOM | 2593 | C | SER | S | 137 | 21.109 | 69.319 | 39.489 | 1.00 | 0.00 |
| ATOM | 2594 | O | SER | S | 137 | 21.481 | 68.414 | 40.226 | 1.00 | 0.00 |
| ATOM | 2595 | CB | SER | S | 137 | 19.625 | 67.772 | 38.109 | 1.00 | 0.00 |
| ATOM | 2596 | OG | SER | S | 137 | 19.118 | 67.612 | 36.767 | 1.00 | 0.00 |
| ATOM | 2597 | H | SER | S | 137 | 21.410 | 69.348 | 36.224 | 1.00 | 0.00 |
| ATOM | 2598 | HG | SER | S | 137 | 19.406 | 66.733 | 36.506 | 1.00 | 0.00 |
| ATOM | 2599 | N | ARG | S | 138 | 21.249 | 70.622 | 39.856 | 1.00 | 0.00 |
| ATOM | 2600 | CA | ARG | S | 138 | 20.552 | 71.746 | 39.222 | 1.00 | 0.00 |
| ATOM | 2601 | C | ARG | S | 138 | 21.464 | 72.960 | 39.049 | 1.00 | 0.00 |
| ATOM | 2602 | O | ARG | S | 138 | 22.674 | 72.866 | 39.260 | 1.00 | 0.00 |
| ATOM | 2603 | CB | ARG | S | 138 | 19.303 | 72.110 | 40.044 | 1.00 | 0.00 |
| ATOM | 2604 | CG | ARG | S | 138 | 18.146 | 71.102 | 39.983 | 1.00 | 0.00 |
| ATOM | 2605 | CD | ARG | S | 138 | 17.701 | 70.824 | 38.547 | 1.00 | 0.00 |
| ATOM | 2606 | NE | ARG | S | 138 | 16.411 | 70.155 | 38.422 | 1.00 | 0.00 |
| ATOM | 2607 | CZ | ARG | S | 138 | 16.057 | 69.593 | 37.243 | 1.00 | 0.00 |
| ATOM | 2608 | NH1 | ARG | S | 138 | 14.797 | 69.271 | 37.043 | 1.00 | 0.00 |
| ATOM | 2609 | NH2 | ARG | S | 138 | 16.956 | 69.348 | 36.300 | 1.00 | 0.00 |
| ATOM | 2610 | H | ARG | S | 138 | 21.808 | 70.756 | 40.667 | 1.00 | 0.00 |

```
ATOM   2611  HE  ARG S 138      15.758  70.094  39.185  1.00  0.00
ATOM   2612 1HH1 ARG S 138      14.540  68.783  36.204  1.00  0.00
ATOM   2613 2HH1 ARG S 138      14.098  69.499  37.723  1.00  0.00
ATOM   2614 1HH2 ARG S 138      16.660  68.923  35.438  1.00  0.00
ATOM   2615 2HH2 ARG S 138      17.934  69.540  36.416  1.00  0.00
ATOM   2616  N   SER S 139      20.851  74.084  38.658  1.00  0.00
ATOM   2617  CA  SER S 139      21.637  75.261  38.315  1.00  0.00
ATOM   2618  C   SER S 139      21.519  76.377  39.321  1.00  0.00
ATOM   2619  O   SER S 139      20.607  76.430  40.153  1.00  0.00
ATOM   2620  CB  SER S 139      21.179  75.779  36.954  1.00  0.00
ATOM   2621  OG  SER S 139      21.000  74.663  36.087  1.00  0.00
ATOM   2622  H   SER S 139      19.872  74.110  38.476  1.00  0.00
ATOM   2623  HG  SER S 139      20.778  75.007  35.214  1.00  0.00
ATOM   2624  N   ASN S 140      22.458  77.324  39.155  1.00  0.00
ATOM   2625  CA  ASN S 140      22.263  78.634  39.775  1.00  0.00
ATOM   2626  C   ASN S 140      20.983  79.271  39.279  1.00  0.00
ATOM   2627  O   ASN S 140      20.497  78.856  38.231  1.00  0.00
ATOM   2628  CB  ASN S 140      23.437  79.558  39.477  1.00  0.00
ATOM   2629  CG  ASN S 140      24.007  80.096  40.771  1.00  0.00
ATOM   2630  OD1 ASN S 140      24.985  79.565  41.293  1.00  0.00
ATOM   2631  ND2 ASN S 140      23.422  81.216  41.215  1.00  0.00
ATOM   2632  OXT ASN S 140      20.428  80.125  39.950  1.00  0.00
ATOM   2633  H   ASN S 140      23.073  77.229  38.378  1.00  0.00
ATOM   2634 1HD2 ASN S 140      23.868  81.821  41.874  1.00  0.00
ATOM   2635 2HD2 ASN S 140      22.509  81.413  40.845  1.00  0.00
END
```

**TABLE 6**

REMARK 1 NMDA Receptor (NR1) Model of the NMDA Receptor Glycine Binding Site

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1 | N | SER | S | 395 | 52.096 | 45.402 | 11.282 | 1.00 | 0.00 |
| ATOM | 2 | CA | SER | S | 395 | 51.059 | 44.524 | 10.749 | 1.00 | 0.00 |
| ATOM | 3 | C | SER | S | 395 | 49.828 | 44.724 | 11.604 | 1.00 | 0.00 |
| ATOM | 4 | O | SER | S | 395 | 49.946 | 45.475 | 12.575 | 1.00 | 0.00 |
| ATOM | 5 | CB | SER | S | 395 | 51.668 | 43.132 | 10.747 | 1.00 | 0.00 |
| ATOM | 6 | OG | SER | S | 395 | 52.996 | 43.307 | 10.216 | 1.00 | 0.00 |
| ATOM | 7 | 1HT | SER | S | 395 | 52.924 | 44.795 | 11.465 | 1.00 | 0.00 |
| ATOM | 8 | 2HT | SER | S | 395 | 51.707 | 46.796 | 12.163 | 1.00 | 0.00 |
| ATOM | 9 | 3HT | SER | S | 395 | 52.293 | 46.139 | 10.585 | 1.00 | 0.00 |
| ATOM | 10 | HG | SER | S | 395 | 53.161 | 42.561 | 9.632 | 1.00 | 0.00 |
| ATOM | 11 | N | THR | S | 396 | 48.702 | 44.106 | 11.210 | 1.00 | 0.00 |
| ATOM | 12 | CA | THR | S | 396 | 47.368 | 44.532 | 11.644 | 1.00 | 0.00 |
| ATOM | 13 | C | THR | S | 396 | 46.429 | 43.338 | 11.572 | 1.00 | 0.00 |
| ATOM | 14 | O | THR | S | 396 | 46.822 | 42.312 | 11.015 | 1.00 | 0.00 |
| ATOM | 15 | CB | THR | S | 396 | 46.892 | 45.651 | 10.698 | 1.00 | 0.00 |
| ATOM | 16 | OG1 | THR | S | 396 | 45.625 | 46.177 | 11.116 | 1.00 | 0.00 |
| ATOM | 17 | CG2 | THR | S | 396 | 46.900 | 45.237 | 9.222 | 1.00 | 0.00 |
| ATOM | 18 | H | THR | S | 396 | 48.694 | 43.421 | 10.485 | 1.00 | 0.00 |
| ATOM | 19 | HG1 | THR | S | 396 | 45.141 | 46.431 | 10.310 | 1.00 | 0.00 |
| ATOM | 20 | N | ARG | S | 397 | 45.213 | 43.502 | 12.120 | 1.00 | 0.00 |
| ATOM | 21 | CA | ARG | S | 397 | 44.211 | 42.491 | 11.797 | 1.00 | 0.00 |
| ATOM | 22 | C | ARG | S | 397 | 43.301 | 42.987 | 10.688 | 1.00 | 0.00 |
| ATOM | 23 | O | ARG | S | 397 | 42.575 | 43.958 | 10.849 | 1.00 | 0.00 |
| ATOM | 24 | CB | ARG | S | 397 | 43.397 | 42.062 | 13.031 | 1.00 | 0.00 |
| ATOM | 25 | CG | ARG | S | 397 | 42.550 | 40.808 | 12.754 | 1.00 | 0.00 |
| ATOM | 26 | CD | ARG | S | 397 | 41.771 | 40.231 | 13.945 | 1.00 | 0.00 |
| ATOM | 27 | NE | ARG | S | 397 | 40.711 | 41.119 | 14.418 | 1.00 | 0.00 |
| ATOM | 28 | CZ | ARG | S | 397 | 39.418 | 40.717 | 14.473 | 1.00 | 0.00 |
| ATOM | 29 | NH1 | ARG | S | 397 | 38.531 | 41.482 | 15.085 | 1.00 | 0.00 |
| ATOM | 30 | NH2 | ARG | S | 397 | 30.034 | 39.560 | 13.949 | 1.00 | 0.00 |
| ATOM | 31 | H | ARG | S | 397 | 44.955 | 44.412 | 12.455 | 1.00 | 0.00 |
| ATOM | 32 | HE | ARG | S | 397 | 40.947 | 42.009 | 14.834 | 1.00 | 0.00 |
| ATOM | 33 | 1HH1 | ARG | S | 397 | 37.566 | 41.219 | 15.196 | 1.00 | 0.00 |
| ATOM | 34 | 2HH1 | ARG | S | 397 | 38.846 | 42.353 | 15.469 | 1.00 | 0.00 |
| ATOM | 35 | 1HH2 | ARG | S | 397 | 38.076 | 39.285 | 13.993 | 1.00 | 0.00 |
| ATOM | 36 | 2HH2 | ARG | S | 397 | 39.694 | 38.954 | 13.515 | 1.00 | 0.00 |
| ATOM | 37 | N | LEU | S | 398 | 43.358 | 42.254 | 9.569 | 1.00 | 0.00 |
| ATOM | 38 | CA | LEU | S | 398 | 42.712 | 42.730 | 8.341 | 1.00 | 0.00 |
| ATOM | 39 | C | LEU | S | 398 | 41.231 | 43.095 | 8.425 | 1.00 | 0.00 |
| ATOM | 40 | O | LEU | S | 398 | 40.691 | 43.892 | 7.656 | 1.00 | 0.00 |
| ATOM | 41 | CB | LEU | S | 398 | 42.995 | 41.770 | 7.180 | 1.00 | 0.00 |
| ATOM | 42 | CG | LEU | S | 398 | 42.801 | 42.406 | 5.796 | 1.00 | 0.00 |
| ATOM | 43 | CD1 | LEU | S | 398 | 43.679 | 43.646 | 5.598 | 1.00 | 0.00 |
| ATOM | 44 | CD2 | LEU | S | 398 | 42.988 | 41.388 | 4.671 | 1.00 | 0.00 |
| ATOM | 45 | H | LEU | S | 398 | 43.930 | 41.439 | 9.600 | 1.00 | 0.00 |
| ATOM | 46 | N | LYS | S | 399 | 40.558 | 42.505 | 9.401 | 1.00 | 0.00 |
| ATOM | 47 | CA | LYS | S | 399 | 39.384 | 43.234 | 9.844 | 1.00 | 0.00 |
| ATOM | 48 | C | LYS | S | 399 | 39.607 | 43.623 | 11.276 | 1.00 | 0.00 |
| ATOM | 49 | O | LYS | S | 399 | 39.963 | 42.795 | 12.108 | 1.00 | 0.00 |
| ATOM | 50 | CB | LYS | S | 399 | 38.123 | 42.405 | 9.620 | 1.00 | 0.00 |
| ATOM | 51 | CG | LYS | S | 399 | 37.663 | 42.587 | 8.171 | 1.00 | 0.00 |
| ATOM | 52 | CD | LYS | S | 399 | 37.023 | 43.962 | 7.950 | 1.00 | 0.00 |
| ATOM | 53 | CE | LYS | S | 399 | 37.403 | 44.644 | 6.640 | 1.00 | 0.00 |
| ATOM | 54 | NZ | LYS | S | 399 | 38.612 | 45.444 | 6.858 | 1.00 | 0.00 |
| ATOM | 55 | H | LYS | S | 399 | 41.008 | 41.880 | 10.032 | 1.00 | 0.00 |
| ATOM | 56 | 1HZ | LYS | S | 399 | 39.403 | 44.644 | 6.640 | 1.00 | 0.00 |
| ATOM | 57 | 2HZ | LYS | S | 399 | 38.914 | 45.814 | 5.938 | 1.00 | 0.00 |
| ATOM | 58 | 3HZ | LYS | S | 399 | 38.403 | 46.254 | 7.479 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 59 | N | ILE | S | 400 | 39.444 | 44.923 | 11.522 | 1.00 | 0.00 |
| ATOM | 60 | CA | ILE | S | 400 | 39.510 | 45.362 | 12.908 | 1.00 | 0.00 |
| ATOM | 61 | C | ILE | S | 400 | 38.075 | 45.496 | 13.355 | 1.00 | 0.00 |
| ATOM | 62 | O | ILE | S | 400 | 37.251 | 46.077 | 12.639 | 1.00 | 0.00 |
| ATOM | 63 | CB | ILE | S | 400 | 40.252 | 46.693 | 13.008 | 1.00 | 0.00 |
| ATOM | 64 | CG1 | ILE | S | 400 | 41.445 | 46.764 | 12.060 | 1.00 | 0.00 |
| ATOM | 65 | CG2 | ILE | S | 400 | 40.697 | 46.955 | 14.447 | 1.00 | 0.00 |
| ATOM | 66 | CD1 | ILE | S | 400 | 41.758 | 48.207 | 11.683 | 1.00 | 0.00 |
| ATOM | 67 | H | ILE | S | 400 | 39.096 | 45.519 | 10.800 | 1.00 | 0.00 |
| ATOM | 68 | N | VAL | S | 401 | 37.789 | 44.837 | 14.479 | 1.00 | 0.00 |
| ATOM | 69 | CA | VAL | S | 401 | 36.403 | 44.863 | 14.896 | 1.00 | 0.00 |
| ATOM | 70 | C | VAL | S | 401 | 36.189 | 45.858 | 15.987 | 1.00 | 0.00 |
| ATOM | 71 | O | VAL | S | 401 | 36.713 | 45.826 | 17.112 | 1.00 | 0.00 |
| ATOM | 72 | CB | VAL | S | 401 | 35.842 | 43.469 | 15.200 | 1.00 | 0.00 |
| ATOM | 73 | CG1 | VAL | S | 401 | 34.470 | 43.486 | 15.885 | 1.00 | 0.00 |
| ATOM | 74 | CG2 | VAL | S | 401 | 35.763 | 42.677 | 13.893 | 1.00 | 0.00 |
| ATOM | 75 | H | VAL | S | 401 | 38.508 | 44.507 | 15.090 | 1.00 | 0.00 |
| ATOM | 76 | N | THR | S | 402 | 35.401 | 46.820 | 15.544 | 1.00 | 0.00 |
| ATOM | 77 | CA | THR | S | 402 | 34.762 | 47.767 | 16.428 | 1.00 | 0.00 |
| ATOM | 78 | C | THR | S | 402 | 33.476 | 47.161 | 16.958 | 1.00 | 0.00 |
| ATOM | 79 | O | THR | S | 402 | 32.429 | 47.216 | 16.319 | 1.00 | 0.00 |
| ATOM | 80 | CB | THR | S | 402 | 34.556 | 49.017 | 15.573 | 1.00 | 0.00 |
| ATOM | 81 | OG1 | THR | S | 402 | 35.855 | 49.585 | 15.313 | 1.00 | 0.00 |
| ATOM | 82 | CG2 | THR | S | 402 | 33.567 | 50.053 | 16.118 | 1.00 | 0.00 |
| ATOM | 83 | H | THR | S | 402 | 35.015 | 46.683 | 14.631 | 1.00 | 0.00 |
| ATOM | 84 | HG1 | THR | S | 402 | 35.666 | 50.435 | 14.894 | 1.00 | 0.00 |
| ATOM | 85 | N | ILE | S | 403 | 33.587 | 46.612 | 18.168 | 1.00 | 0.00 |
| ATOM | 86 | CA | ILE | S | 403 | 32.352 | 46.190 | 18.835 | 1.00 | 0.00 |
| ATOM | 87 | C | ILE | S | 403 | 31.468 | 47.372 | 19.282 | 1.00 | 0.00 |
| ATOM | 88 | O | ILE | S | 403 | 31.956 | 48.481 | 19.519 | 1.00 | 0.00 |
| ATOM | 89 | CB | ILE | S | 403 | 32.733 | 45.186 | 19.934 | 1.00 | 0.00 |
| ATOM | 90 | CG1 | ILE | S | 403 | 31.539 | 44.463 | 20.552 | 1.00 | 0.00 |
| ATOM | 91 | CG2 | ILE | S | 403 | 33.621 | 46.838 | 20.998 | 1.00 | 0.00 |
| ATOM | 92 | CD1 | ILE | S | 403 | 31.919 | 43.134 | 21.200 | 1.00 | 0.00 |
| ATOM | 93 | H | ILE | S | 403 | 34.509 | 46.493 | 18.532 | 1.00 | 0.00 |
| ATOM | 94 | N | HIS | S | 404 | 30.132 | 47.151 | 19.294 | 1.00 | 0.00 |
| ATOM | 95 | CA | HIS | S | 404 | 29.218 | 48.307 | 19.414 | 1.00 | 0.00 |
| ATOM | 96 | C | HIS | S | 404 | 27.998 | 48.146 | 20.329 | 1.00 | 0.00 |
| ATOM | 97 | O | HIS | S | 404 | 27.397 | 47.076 | 20.416 | 1.00 | 0.00 |
| ATOM | 98 | CB | HIS | S | 404 | 28.783 | 48.802 | 18.028 | 1.00 | 0.00 |
| ATOM | 99 | CG | HIS | S | 404 | 28.269 | 50.226 | 18.105 | 1.00 | 0.00 |
| ATOM | 100 | ND1 | HIS | S | 404 | 29.076 | 51.289 | 18.028 | 1.00 | 0.00 |
| ATOM | 101 | CD2 | HIS | S | 404 | 26.961 | 50.687 | 18.277 | 1.00 | 0.00 |
| ATOM | 102 | CE1 | HIS | S | 404 | 28.310 | 52.416 | 18.154 | 1.00 | 0.00 |
| ATOM | 103 | NE2 | HIS | S | 404 | 27.000 | 52.043 | 18.307 | 1.00 | 0.00 |
| ATOM | 104 | H | HIS | S | 404 | 29.790 | 46.223 | 19.131 | 1.00 | 0.00 |
| ATOM | 105 | HD1 | HIS | S | 404 | 30.039 | 51.275 | 17.862 | 1.00 | 0.00 |
| ATOM | 106 | N | GLN | S | 405 | 27.691 | 49.263 | 21.030 | 1.00 | 0.00 |
| ATOM | 107 | CA | GLN | S | 405 | 26.571 | 49.385 | 21.973 | 1.00 | 0.00 |
| ATOM | 108 | C | GLN | S | 405 | 25.195 | 49.355 | 21.296 | 1.00 | 0.00 |
| ATOM | 109 | O | GLN | S | 405 | 25.079 | 49.202 | 20.078 | 1.00 | 0.00 |
| ATOM | 110 | CB | GLN | S | 405 | 26.818 | 50.677 | 22.783 | 1.00 | 0.00 |
| ATOM | 111 | CG | GLN | S | 405 | 26.062 | 51.874 | 24.106 | 1.00 | 0.00 |
| ATOM | 112 | CD | GLN | S | 405 | 26.529 | 52.137 | 24.792 | 1.00 | 0.00 |
| ATOM | 113 | OE1 | GLN | S | 405 | 27.631 | 50.203 | 25.340 | 1.00 | 0.00 |
| ATOM | 114 | NE2 | GLN | S | 405 | 25.655 | 53.154 | 24.741 | 1.00 | 0.00 |
| ATOM | 115 | H | GLN | S | 405 | 28.133 | 50.120 | 20.760 | 1.00 | 0.00 |
| ATOM | 116 | 1HE2 | GLN | S | 405 | 26.863 | 54.087 | 25.037 | 1.00 | 0.00 |
| ATOM | 117 | 2HE2 | GLN | S | 405 | 24.735 | 52.963 | 24.389 | 1.00 | 0.00 |
| ATOM | 118 | N | GLU | S | 406 | 24.133 | 49.462 | 22.121 | 1.00 | 0.00 |
| ATOM | 119 | CA | GLU | S | 406 | 22.864 | 50.027 | 21.635 | 1.00 | 0.00 |
| ATOM | 120 | C | GLU | S | 406 | 22.374 | 51.203 | 22.497 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 121 | O | GLU | S | 406 | 22.385 | 52.362 | 22.071 | 1.00 | 0.00 |
| ATOM | 122 | CB | GLU | S | 406 | 21.813 | 48.912 | 21.402 | 1.00 | 0.00 |
| ATOM | 123 | CG | GLU | S | 406 | 20.436 | 49.288 | 20.825 | 1.00 | 0.00 |
| ATOM | 124 | CD | GLU | S | 406 | 19.628 | 50.208 | 21.736 | 1.00 | 0.00 |
| ATOM | 125 | OE1 | GLU | S | 406 | 19.540 | 51.404 | 21.471 | 1.00 | 0.00 |
| ATOM | 126 | OE2 | GLU | S | 406 | 19.090 | 49.717 | 22.725 | 1.00 | 0.00 |
| ATOM | 127 | H | GLU | S | 406 | 24.221 | 49.248 | 23.091 | 1.00 | 0.00 |
| ATOM | 128 | N | PRO | S | 407 | 21.973 | 50.922 | 23.794 | 1.00 | 0.00 |
| ATOM | 129 | CA | PRO | S | 407 | 21.166 | 51.899 | 24.545 | 1.00 | 0.00 |
| ATOM | 130 | C | PRO | S | 407 | 21.669 | 53.318 | 24.509 | 1.00 | 0.00 |
| ATOM | 131 | O | PRO | S | 407 | 22.894 | 53.552 | 24.589 | 1.00 | 0.00 |
| ATOM | 132 | CB | PRO | S | 407 | 21.112 | 51.327 | 25.962 | 1.00 | 0.00 |
| ATOM | 133 | CG | PRO | S | 407 | 21.173 | 49.822 | 25.751 | 1.00 | 0.00 |
| ATOM | 134 | CD | PRO | S | 407 | 22.159 | 49.708 | 24.598 | 1.00 | 0.00 |
| ATOM | 135 | N | PHE | S | 408 | 20.670 | 54.197 | 24.337 | 1.00 | 0.00 |
| ATOM | 136 | CA | PHE | S | 408 | 20.865 | 55.632 | 24.176 | 1.00 | 0.00 |
| ATOM | 137 | C | PHE | S | 408 | 21.591 | 56.030 | 22.902 | 1.00 | 0.00 |
| ATOM | 138 | O | PHE | S | 408 | 21.002 | 56.632 | 22.003 | 1.00 | 0.00 |
| ATOM | 139 | CB | PHE | S | 408 | 21.440 | 56.250 | 25.460 | 1.00 | 0.00 |
| ATOM | 140 | CG | PHE | S | 408 | 20.345 | 56.433 | 26.493 | 1.00 | 0.00 |
| ATOM | 141 | CD1 | PHE | S | 408 | 19.702 | 55.311 | 27.064 | 1.00 | 0.00 |
| ATOM | 142 | CD2 | PHE | S | 408 | 19.977 | 57.743 | 26.866 | 1.00 | 0.00 |
| ATOM | 143 | CE1 | PHE | S | 408 | 18.674 | 55.503 | 28.007 | 1.00 | 0.00 |
| ATOM | 144 | CE2 | PHE | S | 408 | 18.953 | 57.939 | 27.812 | 1.00 | 0.00 |
| ATOM | 145 | CZ | PHE | S | 408 | 18.309 | 56.816 | 28.371 | 1.00 | 0.00 |
| ATOM | 146 | H | PHE | S | 408 | 19.764 | 53.780 | 24.328 | 1.00 | 0.00 |
| ATOM | 147 | N | VAL | S | 409 | 22.877 | 55.654 | 22.822 | 1.00 | 0.00 |
| ATOM | 148 | CA | VAL | S | 409 | 23.742 | 55.967 | 21.672 | 1.00 | 0.00 |
| ATOM | 149 | C | VAL | S | 409 | 23.322 | 55.384 | 20.319 | 1.00 | 0.00 |
| ATOM | 150 | O | VAL | S | 409 | 23.670 | 54.275 | 19.914 | 1.00 | 0.00 |
| ATOM | 151 | CB | VAL | S | 409 | 25.197 | 55.593 | 22.004 | 1.00 | 0.00 |
| ATOM | 152 | CG1 | VAL | S | 409 | 26.165 | 55.931 | 20.866 | 1.00 | 0.00 |
| ATOM | 153 | CG2 | VAL | S | 409 | 25.635 | 56.250 | 23.316 | 1.00 | 0.00 |
| ATOM | 154 | H | VAL | S | 409 | 23.175 | 55.148 | 23.631 | 1.00 | 0.00 |
| ATOM | 155 | N | TYR | S | 410 | 22.560 | 56.205 | 19.600 | 1.00 | 0.00 |
| ATOM | 156 | CA | TYR | S | 410 | 22.214 | 55.943 | 18.199 | 1.00 | 0.00 |
| ATOM | 157 | C | TYR | S | 410 | 22.277 | 57.294 | 17.529 | 1.00 | 0.00 |
| ATOM | 158 | O | TYR | S | 410 | 22.302 | 58.297 | 18.244 | 1.00 | 0.00 |
| ATOM | 159 | CB | TYR | S | 410 | 20.760 | 55.476 | 18.084 | 1.00 | 0.00 |
| ATOM | 160 | CG | TYR | S | 410 | 20.575 | 53.989 | 17.877 | 1.00 | 0.00 |
| ATOM | 161 | CD1 | TYR | S | 410 | 21.150 | 53.063 | 18.767 | 1.00 | 0.00 |
| ATOM | 162 | CD2 | TYR | S | 410 | 19.763 | 53.572 | 16.804 | 1.00 | 0.00 |
| ATOM | 163 | CE1 | TYR | S | 410 | 20.817 | 51.708 | 18.635 | 1.00 | 0.00 |
| ATOM | 164 | CE2 | TYR | S | 410 | 19.416 | 52.215 | 16.682 | 1.00 | 0.00 |
| ATOM | 165 | CZ | TYR | S | 410 | 19.905 | 51.304 | 17.637 | 1.00 | 0.00 |
| ATOM | 166 | OH | TYR | S | 410 | 19.462 | 49.987 | 17.626 | 1.00 | 0.00 |
| ATOM | 167 | H | TYR | S | 410 | 22.257 | 57.063 | 20.012 | 1.00 | 0.00 |
| ATOM | 168 | HH | TYR | S | 410 | 19.657 | 49.609 | 18.483 | 1.00 | 0.00 |
| ATOM | 169 | N | VAL | S | 411 | 22.218 | 57.306 | 16.181 | 1.00 | 0.00 |
| ATOM | 170 | CA | VAL | S | 411 | 21.470 | 58.411 | 15.562 | 1.00 | 0.00 |
| ATOM | 171 | C | VAL | S | 411 | 20.569 | 57.914 | 14.427 | 1.00 | 0.00 |
| ATOM | 172 | O | VAL | S | 411 | 20.352 | 58.576 | 13.412 | 1.00 | 0.00 |
| ATOM | 173 | CB | VAL | S | 411 | 22.340 | 59.611 | 15.092 | 1.00 | 0.00 |
| ATOM | 174 | CG1 | VAL | S | 411 | 21.500 | 60.892 | 15.035 | 1.00 | 0.00 |
| ATOM | 175 | CG2 | VAL | S | 411 | 23.606 | 59.870 | 15.915 | 1.00 | 0.00 |
| ATOM | 176 | H | VAL | S | 411 | 22.522 | 56.508 | 15.660 | 1.00 | 0.00 |
| ATOM | 177 | N | LYS | S | 412 | 20.080 | 56.662 | 14.624 | 1.00 | 0.00 |
| ATOM | 178 | CA | LYS | S | 412 | 19.066 | 56.134 | 13.700 | 1.00 | 0.00 |
| ATOM | 179 | C | LYS | S | 412 | 17.857 | 55.532 | 14.394 | 1.00 | 0.00 |
| ATOM | 180 | O | LYS | S | 412 | 17.856 | 54.364 | 14.780 | 1.00 | 0.00 |
| ATOM | 181 | CB | LYS | S | 412 | 19.621 | 55.054 | 12.757 | 1.00 | 0.00 |
| ATOM | 182 | CG | LYS | S | 412 | 20.791 | 55.509 | 11.895 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 183 | CD | LYS | S | 412 | 20.442 | 56.701 | 11.019 | 1.00 | 0.00 |
| ATOM | 184 | CE | LYS | S | 412 | 21.665 | 57.550 | 10.696 | 1.00 | 0.00 |
| ATOM | 185 | NZ | LYS | S | 412 | 21.298 | 58.956 | 10.883 | 1.00 | 0.00 |
| ATOM | 186 | H | LYS | S | 412 | 20.306 | 56.130 | 15.434 | 1.00 | 0.00 |
| ATOM | 187 | 1HZ | LYS | S | 412 | 20.602 | 59.227 | 10.154 | 1.00 | 0.00 |
| ATOM | 188 | 2HZ | LYS | S | 412 | 20.890 | 59.098 | 11.832 | 1.00 | 0.00 |
| ATOM | 189 | 3HZ | LYS | S | 412 | 22.129 | 59.568 | 10.768 | 1.00 | 0.00 |
| ATOM | 190 | N | PRO | S | 413 | 16.789 | 56.336 | 14.531 | 1.00 | 0.00 |
| ATOM | 191 | CA | PRO | S | 413 | 15.540 | 55.722 | 14.988 | 1.00 | 0.00 |
| ATOM | 192 | C | PRO | S | 413 | 15.048 | 54.597 | 14.076 | 1.00 | 0.00 |
| ATOM | 193 | O | PRO | S | 413 | 15.549 | 54.355 | 12.980 | 1.00 | 0.00 |
| ATOM | 194 | CB | PRO | S | 413 | 14.598 | 56.929 | 15.105 | 1.00 | 0.00 |
| ATOM | 195 | CG | PRO | S | 413 | 15.188 | 58.026 | 14.217 | 1.00 | 0.00 |
| ATOM | 196 | CD | PRO | S | 413 | 16.690 | 58.767 | 14.266 | 1.00 | 0.00 |
| ATOM | 197 | N | THR | S | 414 | 14.058 | 53.894 | 14.614 | 1.00 | 0.00 |
| ATOM | 198 | CA | THR | S | 414 | 13.363 | 52.857 | 13.860 | 1.00 | 0.00 |
| ATOM | 199 | C | THR | S | 414 | 12.258 | 53.461 | 12.981 | 1.00 | 0.00 |
| ATOM | 200 | O | THR | S | 414 | 11.775 | 54.563 | 13.232 | 1.00 | 0.00 |
| ATOM | 201 | CB | THR | S | 414 | 12.872 | 52.874 | 14.942 | 1.00 | 0.00 |
| ATOM | 202 | OG1 | THR | S | 414 | 14.006 | 51.198 | 15.514 | 1.00 | 0.00 |
| ATOM | 203 | CG2 | THR | S | 414 | 11.803 | 50.863 | 14.529 | 1.00 | 0.00 |
| ATOM | 204 | H | THR | S | 414 | 13.713 | 54.181 | 15.503 | 1.00 | 0.00 |
| ATOM | 205 | HG1 | THR | S | 414 | 14.458 | 50.787 | 14.783 | 1.00 | 0.00 |
| ATOM | 206 | N | LEU | S | 415 | 11.870 | 52.705 | 11.919 | 1.00 | 0.00 |
| ATOM | 207 | CA | LEU | S | 415 | 10.645 | 52.927 | 11.117 | 1.00 | 0.00 |
| ATOM | 208 | C | LEU | S | 415 | 10.671 | 52.092 | 9.855 | 1.00 | 0.00 |
| ATOM | 209 | O | LEU | S | 415 | 11.5254 | 52.321 | 9.002 | 1.00 | 0.00 |
| ATOM | 210 | CB | LEU | S | 415 | 10.426 | 54.382 | 10.659 | 1.00 | 0.00 |
| ATOM | 211 | CG | LEU | S | 415 | 9.083 | 54.658 | 9.975 | 1.00 | 0.00 |
| ATOM | 212 | CD1 | LEU | S | 415 | 7.896 | 54.403 | 10.907 | 1.00 | 0.00 |
| ATOM | 213 | CD2 | LEU | S | 415 | 9.047 | 56.058 | 9.362 | 1.00 | 0.00 |
| ATOM | 214 | H | LEU | S | 415 | 12.451 | 51.915 | 11.704 | 1.00 | 0.00 |
| ATOM | 215 | N | SER | S | 416 | 9.736 | 51.143 | 9.773 | 1.00 | 0.00 |
| ATOM | 216 | CA | SER | S | 416 | 9.682 | 50.278 | 8.595 | 1.00 | 0.00 |
| ATOM | 217 | C | SER | S | 416 | 9.584 | 51.018 | 7.269 | 1.00 | 0.00 |
| ATOM | 218 | O | SER | S | 416 | 8.576 | 51.657 | 6.968 | 1.00 | 0.00 |
| ATOM | 219 | CB | SER | S | 416 | 8.497 | 49.322 | 8.734 | 1.00 | 0.00 |
| ATOM | 220 | OG | SER | S | 416 | 7.999 | 49.337 | 10.085 | 1.00 | 0.00 |
| ATOM | 221 | H | SER | S | 416 | 9.075 | 50.986 | 10.500 | 1.00 | 0.00 |
| ATOM | 222 | HG | SER | S | 416 | 8.319 | 48.530 | 10.477 | 1.00 | 0.00 |
| ATOM | 223 | N | ASP | S | 417 | 10.669 | 50.915 | 6.495 | 1.00 | 0.00 |
| ATOM | 224 | CA | ASP | S | 417 | 10.643 | 51.523 | 5.164 | 1.00 | 0.00 |
| ATOM | 225 | C | ASP | S | 417 | 11.648 | 50.824 | 4.281 | 1.00 | 0.00 |
| ATOM | 226 | O | ASP | S | 417 | 12.724 | 50.435 | 4.725 | 1.00 | 0.00 |
| ATOM | 227 | CB | ASP | S | 417 | 10.895 | 53.050 | 5.235 | 1.00 | 0.00 |
| ATOM | 228 | CG | ASP | S | 417 | 10.978 | 53.757 | 3.878 | 1.00 | 0.00 |
| ATOM | 229 | OD1 | ASP | S | 417 | 11.611 | 54.802 | 3.760 | 1.00 | 0.00 |
| ATOM | 230 | OD2 | ASP | S | 417 | 10.406 | 53.299 | 2.901 | 1.00 | 0.00 |
| ATOM | 231 | H | ASP | S | 417 | 11.369 | 50.242 | 6.752 | 1.00 | 0.00 |
| ATOM | 232 | N | GLY | S | 418 | 11.247 | 50.700 | 3.008 | 1.00 | 0.00 |
| ATOM | 233 | CA | GLY | S | 418 | 12.141 | 50.155 | 1.996 | 1.00 | 0.00 |
| ATOM | 234 | C | GLY | S | 418 | 12.789 | 51.216 | 1.114 | 1.00 | 0.00 |
| ATOM | 235 | O | GLY | S | 418 | 12.346 | 51.487 | 0.002 | 1.00 | 0.00 |
| ATOM | 236 | H | GLY | S | 418 | 10.404 | 51.175 | 2.754 | 1.00 | 0.00 |
| ATOM | 237 | N | THR | S | 419 | 13.852 | 51.825 | 1.653 | 1.00 | 0.00 |
| ATOM | 238 | CA | THR | S | 419 | 14.633 | 52.758 | 0.830 | 1.00 | 0.00 |
| ATOM | 239 | C | THR | S | 419 | 16.137 | 52.803 | 1.175 | 1.00 | 0.00 |
| ATOM | 240 | O | THR | S | 419 | 16.692 | 53.865 | 1.447 | 1.00 | 0.00 |
| ATOM | 241 | CB | THR | S | 419 | 14.020 | 54.177 | 0.889 | 1.00 | 0.00 |
| ATOM | 242 | OG1 | THR | S | 419 | 12.585 | 54.172 | 1.074 | 1.00 | 0.00 |
| ATOM | 243 | CG2 | THR | S | 419 | 14.377 | 54.962 | -0.376 | 1.00 | 0.00 |
| ATOM | 244 | H | THR | S | 419 | 14.133 | 51.449 | 2.533 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 245 | HG1 | THR | S | 419 | 12.416 | 53.567 | 1.800 | 1.00 | 0.00 |
| ATOM | 246 | N | CYS | S | 420 | 16.751 | 51.596 | 1.245 | 1.00 | 0.00 |
| ATOM | 247 | CA | CYS | S | 420 | 17.931 | 51.309 | 2.101 | 1.00 | 0.00 |
| ATOM | 248 | C | CYS | S | 420 | 17.575 | 51.314 | 3.575 | 1.00 | 0.00 |
| ATOM | 249 | O | CYS | S | 420 | 18.385 | 51.101 | 4.475 | 1.00 | 0.00 |
| ATOM | 250 | CB | CYS | S | 420 | 19.139 | 52.246 | 2.015 | 1.00 | 0.00 |
| ATOM | 251 | SG | CYS | S | 420 | 19.996 | 52.479 | 0.436 | 1.00 | 0.00 |
| ATOM | 252 | H | CYS | S | 420 | 16.219 | 50.778 | 1.018 | 1.00 | 0.00 |
| ATOM | 253 | N | LYS | S | 421 | 16.301 | 51.651 | 3.765 | 1.00 | 0.00 |
| ATOM | 254 | CA | LYS | S | 421 | 15.770 | 52.085 | 5.038 | 1.00 | 0.00 |
| ATOM | 255 | C | LYS | S | 421 | 15.290 | 50.911 | 5.848 | 1.00 | 0.00 |
| ATOM | 256 | O | LYS | S | 421 | 14.875 | 51.081 | 6.993 | 1.00 | 0.00 |
| ATOM | 257 | CB | LYS | S | 421 | 14.625 | 53.059 | 4.796 | 1.00 | 0.00 |
| ATOM | 258 | CG | LYS | S | 421 | 14.910 | 54.493 | 5.226 | 1.00 | 0.00 |
| ATOM | 259 | CD | LYS | S | 421 | 13.824 | 55.099 | 6.128 | 1.00 | 0.00 |
| ATOM | 260 | CE | LYS | S | 421 | 13.713 | 54.545 | 7.559 | 1.00 | 0.00 |
| ATOM | 261 | NZ | LYS | S | 421 | 13.349 | 53.126 | 7.608 | 1.00 | 0.00 |
| ATOM | 262 | H | LYS | S | 421 | 15.721 | 51.239 | 3.072 | 1.00 | 0.00 |
| ATOM | 263 | 1HZ | LYS | S | 421 | 14.078 | 52.502 | 7.219 | 1.00 | 0.00 |
| ATOM | 264 | 2HZ | LYS | S | 421 | 13.218 | 52.821 | 8.596 | 1.00 | 0.00 |
| ATOM | 265 | 3HZ | LYS | S | 421 | 12.440 | 52.948 | 7.143 | 1.00 | 0.00 |
| ATOM | 266 | N | GLU | S | 422 | 15.423 | 49.741 | 5.199 | 1.00 | 0.00 |
| ATOM | 267 | CA | GLU | S | 422 | 15.427 | 48.435 | 5.831 | 1.00 | 0.00 |
| ATOM | 268 | C | GLU | S | 422 | 16.498 | 48.409 | 6.903 | 1.00 | 0.00 |
| ATOM | 269 | O | GLU | S | 422 | 17.058 | 49.433 | 7.302 | 1.00 | 0.00 |
| ATOM | 270 | CB | GLU | S | 422 | 15.728 | 47.341 | 4.787 | 1.00 | 0.00 |
| ATOM | 271 | CG | GLU | S | 422 | 15.036 | 47.402 | 3.415 | 1.00 | 0.00 |
| ATOM | 272 | CD | GLU | S | 422 | 15.715 | 48.421 | 2.512 | 1.00 | 0.00 |
| ATOM | 273 | OE1 | GLU | S | 422 | 16.902 | 48.307 | 2.251 | 1.00 | 0.00 |
| ATOM | 274 | OE2 | GLU | S | 422 | 15.067 | 49.359 | 2.079 | 1.00 | 0.00 |
| ATOM | 275 | H | GLU | S | 422 | 15.655 | 49.758 | 4.231 | 1.00 | 0.00 |
| ATOM | 276 | N | GLU | S | 423 | 16.870 | 47.201 | 7.327 | 1.00 | 0.00 |
| ATOM | 277 | CA | GLU | S | 423 | 18.017 | 47.245 | 8.226 | 1.00 | 0.00 |
| ATOM | 278 | C | GLU | S | 423 | 19.397 | 47.456 | 7.596 | 1.00 | 0.00 |
| ATOM | 279 | O | GLU | S | 423 | 20.422 | 46.949 | 8.066 | 1.00 | 0.00 |
| ATOM | 280 | CB | GLU | S | 423 | 17.924 | 46.085 | 9.202 | 1.00 | 0.00 |
| ATOM | 281 | CG | GLU | S | 423 | 16.686 | 46.302 | 10.084 | 1.00 | 0.00 |
| ATOM | 282 | CD | GLU | S | 423 | 16.050 | 44.979 | 10.448 | 1.00 | 0.00 |
| ATOM | 283 | OE1 | GLU | S | 423 | 14.842 | 44.925 | 10.644 | 1.00 | 0.00 |
| ATOM | 284 | OE2 | GLU | S | 423 | 16.751 | 43.980 | 10.511 | 1.00 | 0.00 |
| ATOM | 285 | H | GLU | S | 423 | 16.440 | 46.353 | 7.014 | 1.00 | 0.00 |
| ATOM | 286 | N | PHE | S | 424 | 19.410 | 48.313 | 6.556 | 1.00 | 0.00 |
| ATOM | 287 | CA | PHE | S | 424 | 20.644 | 49.002 | 6.180 | 1.00 | 0.00 |
| ATOM | 288 | C | PHE | S | 424 | 20.620 | 50.448 | 6.663 | 1.00 | 0.00 |
| ATOM | 289 | O | PHE | S | 424 | 20.782 | 51.418 | 5.920 | 1.00 | 0.00 |
| ATOM | 290 | CB | PHE | S | 424 | 20.874 | 48.888 | 4.669 | 1.00 | 0.00 |
| ATOM | 291 | CG | PHE | S | 424 | 20.787 | 47.435 | 4.254 | 1.00 | 0.00 |
| ATOM | 292 | CD1 | PHE | S | 424 | 19.642 | 46.987 | 3.559 | 1.00 | 0.00 |
| ATOM | 293 | CD2 | PHE | S | 424 | 21.836 | 46.547 | 4.582 | 1.00 | 0.00 |
| ATOM | 294 | CE1 | PHE | S | 424 | 19.532 | 45.628 | 3.207 | 1.00 | 0.00 |
| ATOM | 295 | CE2 | PHE | S | 424 | 21.728 | 45.188 | 4.230 | 1.00 | 0.00 |
| ATOM | 296 | CZ | PHE | S | 424 | 20.573 | 44.741 | 3.554 | 1.00 | 0.00 |
| ATOM | 297 | H | PHE | S | 424 | 18.552 | 48.618 | 6.144 | 1.00 | 0.00 |
| ATOM | 298 | N | THR | S | 425 | 20.353 | 50.501 | 7.982 | 1.00 | 0.00 |
| ATOM | 299 | CA | THR | S | 425 | 20.344 | 51.707 | 8.809 | 1.00 | 0.00 |
| ATOM | 300 | C | THR | S | 425 | 19.357 | 52.795 | 8.354 | 1.00 | 0.00 |
| ATOM | 301 | O | THR | S | 425 | 18.267 | 52.508 | 7.845 | 1.00 | 0.00 |
| ATOM | 302 | CB | THR | S | 425 | 21.818 | 52.127 | 9.141 | 1.00 | 0.00 |
| ATOM | 303 | OG1 | THR | S | 425 | 21.868 | 53.076 | 10.220 | 1.00 | 0.00 |
| ATOM | 304 | CG2 | THR | S | 425 | 22.700 | 52.620 | 7.988 | 1.00 | 0.00 |
| ATOM | 305 | H | THR | S | 425 | 20.169 | 49.642 | 8.438 | 1.00 | 0.00 |
| ATOM | 306 | HG1 | THR | S | 425 | 22.740 | 53.015 | 10.620 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 307 | N | VAL | S | 426 | 19.765 | 54.075 | 8.537 | 1.00 | 0.00 |
| ATOM | 308 | CA | VAL | S | 426 | 19.192 | 55.285 | 7.915 | 1.00 | 0.00 |
| ATOM | 309 | C | VAL | S | 426 | 17.720 | 55.627 | 8.135 | 1.00 | 0.00 |
| ATOM | 310 | O | VAL | S | 426 | 16.800 | 55.153 | 7.477 | 1.00 | 0.00 |
| ATOM | 311 | CB | VAL | S | 426 | 19.619 | 55.464 | 6.439 | 1.00 | 0.00 |
| ATOM | 312 | CG1 | VAL | S | 426 | 21.138 | 55.608 | 6.353 | 1.00 | 0.00 |
| ATOM | 313 | CG2 | VAL | S | 426 | 19.093 | 54.409 | 5.459 | 1.00 | 0.00 |
| ATOM | 314 | H | VAL | S | 426 | 20.528 | 54.160 | 9.182 | 1.00 | 0.00 |
| ATOM | 315 | N | ASN | S | 427 | 17.481 | 56.489 | 9.132 | 1.00 | 0.00 |
| ATOM | 316 | CA | ASN | S | 427 | 16.081 | 56.864 | 9.312 | 1.00 | 0.00 |
| ATOM | 317 | C | ASN | S | 427 | 15.745 | 58.181 | 8.660 | 1.00 | 0.00 |
| ATOM | 318 | O | ASN | S | 427 | 15.441 | 59.194 | 9.279 | 1.00 | 0.00 |
| ATOM | 319 | CB | ASN | S | 427 | 15.647 | 56.835 | 10.771 | 1.00 | 0.00 |
| ATOM | 320 | CG | ASN | S | 427 | 14.140 | 56.648 | 10.852 | 1.00 | 0.00 |
| ATOM | 321 | OD1 | ASN | S | 427 | 13.328 | 57.557 | 10.717 | 1.00 | 0.00 |
| ATOM | 322 | ND2 | ASN | S | 427 | 13.775 | 55.404 | 11.120 | 1.00 | 0.00 |
| ATOM | 323 | H | ASN | S | 427 | 18.205 | 56.991 | 9.601 | 1.00 | 0.00 |
| ATOM | 324 | 1HD2 | ASN | S | 427 | 12.828 | 55.112 | 11.193 | 1.00 | 0.00 |
| ATOM | 325 | 2HD2 | ASN | S | 427 | 14.474 | 54.721 | 11.359 | 1.00 | 0.00 |
| ATOM | 326 | N | GLY | S | 428 | 15.832 | 58.118 | 7.324 | 1.00 | 0.00 |
| ATOM | 327 | CA | GLY | S | 428 | 15.545 | 59.339 | 6.572 | 1.00 | 0.00 |
| ATOM | 328 | C | GLY | S | 428 | 16.706 | 59.866 | 5.745 | 1.00 | 0.00 |
| ATOM | 329 | O | GLY | S | 428 | 16.518 | 60.393 | 4.652 | 1.00 | 0.00 |
| ATOM | 330 | H | GLY | S | 428 | 16.117 | 57.251 | 6.911 | 1.00 | 0.00 |
| ATOM | 331 | N | ASP | S | 429 | 17.901 | 59.671 | 6.303 | 1.00 | 0.00 |
| ATOM | 332 | CA | ASP | S | 429 | 19.165 | 60.117 | 5.707 | 1.00 | 0.00 |
| ATOM | 333 | C | ASP | S | 429 | 19.322 | 60.195 | 4.169 | 1.00 | 0.00 |
| ATOM | 334 | O | ASP | S | 429 | 19.755 | 61.223 | 3.652 | 1.00 | 0.00 |
| ATOM | 335 | CB | ASP | S | 429 | 20.340 | 59.381 | 6.391 | 1.00 | 0.00 |
| ATOM | 336 | CG | ASP | S | 429 | 20.179 | 59.330 | 7.912 | 1.00 | 0.00 |
| ATOM | 337 | OD1 | ASP | S | 429 | 20.760 | 60.141 | 8.610 | 1.00 | 0.00 |
| ATOM | 338 | OD2 | ASP | S | 429 | 19.474 | 58.476 | 8.432 | 1.00 | 0.00 |
| ATOM | 339 | H | ASP | S | 429 | 17.940 | 59.272 | 7.221 | 1.00 | 0.00 |
| ATOM | 340 | N | PRO | S | 430 | 18.977 | 59.108 | 3.407 | 1.00 | 0.00 |
| ATOM | 341 | CA | PRO | S | 430 | 19.189 | 59.190 | 1.954 | 1.00 | 0.00 |
| ATOM | 342 | C | PRO | S | 430 | 18.112 | 59.916 | 1.142 | 1.00 | 0.00 |
| ATOM | 343 | O | PRO | S | 430 | 18.195 | 59.941 | -0.089 | 1.00 | 0.00 |
| ATOM | 344 | CB | PRO | S | 430 | 19.292 | 57.713 | 1.569 | 1.00 | 0.00 |
| ATOM | 345 | CG | PRO | S | 430 | 18.302 | 57.020 | 2.500 | 1.00 | 0.00 |
| ATOM | 346 | CD | PRO | S | 430 | 18.502 | 57.780 | 3.806 | 1.00 | 0.00 |
| ATOM | 347 | N | VAL | S | 431 | 17.106 | 60.464 | 1.854 | 1.00 | 0.00 |
| ATOM | 348 | CA | VAL | S | 431 | 15.979 | 61.241 | 1.309 | 1.00 | 0.00 |
| ATOM | 349 | C | VAL | S | 431 | 15.178 | 60.628 | 0.153 | 1.00 | 0.00 |
| ATOM | 350 | O | VAL | S | 431 | 14.934 | 61.240 | -0.887 | 1.00 | 0.00 |
| ATOM | 351 | CB | VAL | S | 431 | 16.395 | 62.704 | 1.029 | 1.00 | 0.00 |
| ATOM | 352 | CG1 | VAL | S | 431 | 15.181 | 63.641 | 0.982 | 1.00 | 0.00 |
| ATOM | 353 | CG2 | VAL | S | 431 | 17.394 | 63.223 | 2.070 | 1.00 | 0.00 |
| ATOM | 354 | H | VAL | S | 431 | 17.215 | 60.463 | 2.847 | 1.00 | 0.00 |
| ATOM | 355 | N | LYS | S | 432 | 14.778 | 59.368 | 0.422 | 1.00 | 0.00 |
| ATOM | 356 | CA | LYS | S | 432 | 13.988 | 58.604 | -0.554 | 1.00 | 0.00 |
| ATOM | 357 | C | LYS | S | 432 | 14.414 | 58.683 | -2.007 | 1.00 | 0.00 |
| ATOM | 358 | O | LYS | S | 432 | 13.655 | 58.942 | -2.945 | 1.00 | 0.00 |
| ATOM | 359 | CB | LYS | S | 432 | 12.488 | 58.841 | -0.398 | 1.00 | 0.00 |
| ATOM | 360 | CG | LYS | S | 432 | 11.961 | 58.007 | 0.764 | 1.00 | 0.00 |
| ATOM | 361 | CD | LYS | S | 432 | 10.439 | 57.890 | 0.750 | 1.00 | 0.00 |
| ATOM | 362 | CE | LYS | S | 432 | 9.951 | 56.912 | 1.827 | 1.00 | 0.00 |
| ATOM | 363 | NZ | LYS | S | 432 | 10.465 | 55.565 | 1.558 | 1.00 | 0.00 |
| ATOM | 364 | H | LYS | S | 432 | 14.920 | 59.025 | 1.348 | 1.00 | 0.00 |
| ATOM | 365 | 1HZ | LYS | S | 432 | 10.012 | 55.053 | 0.786 | 1.00 | 0.00 |
| ATOM | 366 | 2HZ | LYS | S | 432 | 11.494 | 55.526 | 1.420 | 1.00 | 0.00 |
| ATOM | 367 | 3HZ | LYS | S | 432 | 10.322 | 55.004 | 2.422 | 1.00 | 0.00 |
| ATOM | 368 | N | LYS | S | 433 | 15.714 | 58.424 | -2.125 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 369 | CA | LYS | S | 433 | 16.468 | 58.425 | -3.362 | 1.00 | 0.00 |
| ATOM | 370 | C | LYS | S | 433 | 17.429 | 57.278 | -3.157 | 1.00 | 0.00 |
| ATOM | 371 | O | LYS | S | 433 | 18.012 | 57.174 | -2.079 | 1.00 | 0.00 |
| ATOM | 372 | CB | LYS | S | 433 | 17.208 | 59.766 | -3.408 | 1.00 | 0.00 |
| ATOM | 373 | CG | LYS | S | 433 | 18.466 | 59.883 | -4.277 | 1.00 | 0.00 |
| ATOM | 374 | CD | LYS | S | 433 | 19.546 | 60.703 | -3.552 | 1.00 | 0.00 |
| ATOM | 375 | CE | LYS | S | 433 | 20.574 | 59.895 | -2.735 | 1.00 | 0.00 |
| ATOM | 376 | NZ | LYS | S | 433 | 19.939 | 58.838 | -1.940 | 1.00 | 0.00 |
| ATOM | 377 | H | LYS | S | 433 | 16.196 | 58.262 | -1.270 | 1.00 | 0.00 |
| ATOM | 378 | 1HZ | LYS | S | 433 | 19.167 | 59.202 | -1.344 | 1.00 | 0.00 |
| ATOM | 379 | 2HZ | LYS | S | 433 | 19.536 | 58.130 | -2.591 | 1.00 | 0.00 |
| ATOM | 380 | 3HZ | LYS | S | 433 | 20.624 | 58.294 | -1.380 | 1.00 | 0.00 |
| ATOM | 381 | N | VAL | S | 434 | 17.596 | 56.438 | -4.191 | 1.00 | 0.00 |
| ATOM | 382 | CA | VAL | S | 434 | 18.563 | 55.338 | -4.051 | 1.00 | 0.00 |
| ATOM | 383 | C | VAL | S | 434 | 19.957 | 55.798 | -3.629 | 1.00 | 0.00 |
| ATOM | 384 | O | VAL | S | 434 | 20.252 | 56.988 | -3.706 | 1.00 | 0.00 |
| ATOM | 385 | CB | VAL | S | 434 | 18.627 | 54.505 | -5.339 | 1.00 | 0.00 |
| ATOM | 386 | CG1 | VAL | S | 434 | 17.290 | 53.803 | -5.586 | 1.00 | 0.00 |
| ATOM | 387 | CG2 | VAL | S | 434 | 19.080 | 55.335 | -6.546 | 1.00 | 0.00 |
| ATOM | 388 | H | VAL | S | 434 | 17.088 | 56.581 | -5.404 | 1.00 | 0.00 |
| ATOM | 389 | N | ILE | S | 435 | 20.768 | 54.823 | -3.174 | 1.00 | 0.00 |
| ATOM | 390 | CA | ILE | S | 435 | 22.084 | 55.095 | -2.574 | 1.00 | 0.00 |
| ATOM | 391 | C | ILE | S | 435 | 22.014 | 55.733 | -1.182 | 1.00 | 0.00 |
| ATOM | 392 | O | ILE | S | 435 | 21.319 | 56.722 | -0.936 | 1.00 | 0.00 |
| ATOM | 393 | CB | ILE | S | 435 | 23.006 | 55.869 | -3.548 | 1.00 | 0.00 |
| ATOM | 394 | CG1 | ILE | S | 435 | 23.113 | 55.120 | -4.881 | 1.00 | 0.00 |
| ATOM | 395 | CG2 | ILE | S | 435 | 24.406 | 56.088 | -2.968 | 1.00 | 0.00 |
| ATOM | 396 | CD1 | ILE | S | 435 | 23.832 | 55.926 | -5.965 | 1.00 | 0.00 |
| ATOM | 397 | H | ILE | S | 435 | 20.448 | 53.879 | -3.220 | 1.00 | 0.00 |
| ATOM | 398 | N | CYS | S | 436 | 22.756 | 55.067 | -0.275 | 1.00 | 0.00 |
| ATOM | 399 | CA | CYS | S | 436 | 22.787 | 55.381 | 1.163 | 1.00 | 0.00 |
| ATOM | 400 | C | CYS | S | 436 | 24.204 | 55.415 | 1.748 | 1.00 | 0.00 |
| ATOM | 401 | O | CYS | S | 436 | 24.475 | 55.161 | 2.927 | 1.00 | 0.00 |
| ATOM | 402 | CB | CYS | S | 436 | 21.904 | 54.368 | 1.902 | 1.00 | 0.00 |
| ATOM | 403 | SG | CYS | S | 436 | 21.915 | 52.736 | 1.091 | 1.00 | 0.00 |
| ATOM | 404 | H | CYS | S | 436 | 23.269 | 54.268 | -0.896 | 1.00 | 0.00 |
| ATOM | 405 | N | THR | S | 437 | 25.134 | 55.710 | 0.828 | 1.00 | 0.00 |
| ATOM | 406 | CA | THR | S | 437 | 26.520 | 55.830 | 1.262 | 1.00 | 0.00 |
| ATOM | 407 | C | THR | S | 437 | 26.738 | 57.171 | 1.935 | 1.00 | 0.00 |
| ATOM | 408 | O | THR | S | 437 | 26.437 | 58.204 | 1.340 | 1.00 | 0.00 |
| ATOM | 409 | CB | THR | S | 437 | 27.401 | 55.681 | 0.023 | 1.00 | 0.00 |
| ATOM | 410 | OG1 | THR | S | 437 | 26.904 | 56.531 | -1.030 | 1.00 | 0.00 |
| ATOM | 411 | CG2 | THR | S | 437 | 27.440 | 54.227 | -0.454 | 1.00 | 0.00 |
| ATOM | 412 | H | THR | S | 437 | 24.910 | 55.969 | -0.109 | 1.00 | 0.00 |
| ATOM | 413 | HG1 | THR | S | 437 | 27.186 | 57.409 | -0.758 | 1.00 | 0.00 |
| ATOM | 414 | N | GLY | S | 438 | 27.240 | 57.094 | 3.170 | 1.00 | 0.00 |
| ATOM | 415 | CA | GLY | S | 438 | 27.493 | 58.326 | 3.910 | 1.00 | 0.00 |
| ATOM | 416 | C | GLY | S | 438 | 27.728 | 57.984 | 5.363 | 1.00 | 0.00 |
| ATOM | 417 | O | GLY | S | 438 | 28.852 | 57.682 | 5.773 | 1.00 | 0.00 |
| ATOM | 418 | H | GLY | S | 438 | 27.398 | 56.203 | 3.595 | 1.00 | 0.00 |
| ATOM | 419 | N | PRO | S | 439 | 26.582 | 57.976 | 6.097 | 1.00 | 0.00 |
| ATOM | 420 | CA | PRO | S | 439 | 26.538 | 57.446 | 7.466 | 1.00 | 0.00 |
| ATOM | 421 | C | PRO | S | 439 | 27.436 | 56.236 | 7.679 | 1.00 | 0.00 |
| ATOM | 422 | O | PRO | S | 439 | 27.375 | 55.253 | 6.935 | 1.00 | 0.00 |
| ATOM | 423 | CB | PRO | S | 439 | 25.043 | 57.146 | 7.614 | 1.00 | 0.00 |
| ATOM | 424 | CG | PRO | S | 439 | 24.365 | 58.283 | 6.857 | 1.00 | 0.00 |
| ATOM | 425 | CD | PRO | S | 439 | 25.275 | 58.452 | 5.647 | 1.00 | 0.00 |
| ATOM | 426 | N | ASN | S | 440 | 28.315 | 56.338 | 8.663 | 1.00 | 0.00 |
| ATOM | 427 | CA | ASN | S | 440 | 29.293 | 55.263 | 8.781 | 1.00 | 0.00 |
| ATOM | 428 | C | ASN | S | 440 | 28.921 | 54.239 | 9.817 | 1.00 | 0.00 |
| ATOM | 429 | O | ASN | S | 440 | 29.223 | 54.368 | 11.000 | 1.00 | 0.00 |
| ATOM | 430 | CB | ASN | S | 440 | 30.695 | 55.801 | 9.037 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 431 | CG | ASN | S | 440 | 31.726 | 54.732 | 8.723 | 1.00 | 0.00 |
| ATOM | 432 | OD1 | ASN | S | 440 | 31.882 | 54.249 | 7.602 | 1.00 | 0.00 |
| ATOM | 433 | ND2 | ASN | S | 440 | 32.475 | 54.381 | 9.762 | 1.00 | 0.00 |
| ATOM | 434 | H | ASN | S | 440 | 28.321 | 57.134 | 9.275 | 1.00 | 0.00 |
| ATOM | 435 | 1HD2 | ASN | S | 440 | 32.113 | 54.732 | 10.634 | 1.00 | 0.00 |
| ATOM | 436 | 2HD2 | ASN | S | 440 | 33.312 | 53.835 | 9.685 | 1.00 | 0.00 |
| ATOM | 437 | N | ASP | S | 441 | 28.243 | 53.209 | 9.296 | 1.00 | 0.00 |
| ATOM | 438 | CA | ASP | S | 441 | 27.613 | 52.210 | 10.158 | 1.00 | 0.00 |
| ATOM | 439 | C | ASP | S | 441 | 28.489 | 51.533 | 11.213 | 1.00 | 0.00 |
| ATOM | 440 | O | ASP | S | 441 | 29.727 | 51.544 | 11.199 | 1.00 | 0.00 |
| ATOM | 441 | CB | ASP | S | 441 | 26.874 | 51.203 | 9.260 | 1.00 | 0.00 |
| ATOM | 442 | CG | ASP | S | 441 | 25.926 | 50.355 | 10.084 | 1.00 | 0.00 |
| ATOM | 443 | OD1 | ASP | S | 441 | 24.823 | 50.798 | 10.368 | 1.00 | 0.00 |
| ATOM | 444 | OD2 | ASP | S | 441 | 26.324 | 49.273 | 10.492 | 1.00 | 0.00 |
| ATOM | 445 | H | ASP | S | 441 | 27.919 | 53.289 | 8.354 | 1.00 | 0.00 |
| ATOM | 446 | N | THR | S | 442 | 27.790 | 50.907 | 12.174 | 1.00 | 0.00 |
| ATOM | 447 | CA | THR | S | 442 | 28.520 | 50.437 | 13.332 | 1.00 | 0.00 |
| ATOM | 448 | C | THR | S | 442 | 28.058 | 49.111 | 13.953 | 1.00 | 0.00 |
| ATOM | 449 | O | THR | S | 442 | 28.868 | 48.363 | 14.488 | 1.00 | 0.00 |
| ATOM | 450 | CB | THR | S | 442 | 28.559 | 51.628 | 14.291 | 1.00 | 0.00 |
| ATOM | 451 | OG1 | THR | S | 442 | 29.603 | 51.528 | 15.271 | 1.00 | 0.00 |
| ATOM | 452 | CG2 | THR | S | 442 | 27.199 | 51.938 | 14.896 | 1.00 | 0.00 |
| ATOM | 453 | H | THR | S | 442 | 26.792 | 50.817 | 12.125 | 1.00 | 0.00 |
| ATOM | 454 | HG1 | THR | S | 442 | 29.628 | 60.607 | 15.537 | 1.00 | 0.00 |
| ATOM | 455 | N | SER | S | 443 | 26.754 | 48.820 | 13.868 | 1.00 | 0.00 |
| ATOM | 456 | CA | SER | S | 443 | 26.224 | 47.609 | 14.514 | 1.00 | 0.00 |
| ATOM | 457 | C | SER | S | 443 | 24.941 | 47.097 | 13.874 | 1.00 | 0.00 |
| ATOM | 458 | O | SER | S | 443 | 23.839 | 47.599 | 14.115 | 1.00 | 0.00 |
| ATOM | 459 | CB | SER | S | 443 | 25.966 | 47.837 | 16.017 | 1.00 | 0.00 |
| ATOM | 460 | OG | SER | S | 443 | 25.936 | 46.627 | 16.817 | 1.00 | 0.00 |
| ATOM | 461 | H | SER | S | 443 | 26.138 | 49.443 | 13.832 | 1.00 | 0.00 |
| ATOM | 462 | HG | SER | S | 443 | 25.700 | 45.922 | 16.209 | 1.00 | 0.00 |
| ATOM | 463 | N | PRO | S | 444 | 25.103 | 46.024 | 13.076 | 1.00 | 0.00 |
| ATOM | 464 | CA | PRO | S | 444 | 23.943 | 45.248 | 12.631 | 1.00 | 0.00 |
| ATOM | 465 | C | PRO | S | 444 | 23.310 | 44.412 | 13.742 | 1.00 | 0.00 |
| ATOM | 466 | O | PRO | S | 444 | 23.596 | 43.223 | 13.913 | 1.00 | 0.00 |
| ATOM | 467 | CB | PRO | S | 444 | 24.542 | 44.413 | 11.494 | 1.00 | 0.00 |
| ATOM | 468 | CG | PRO | S | 444 | 26.003 | 44.194 | 11.876 | 1.00 | 0.00 |
| ATOM | 469 | CD | PRO | S | 444 | 26.367 | 45.496 | 12.576 | 1.00 | 0.00 |
| ATOM | 470 | N | GLY | S | 445 | 22.433 | 45.108 | 14.488 | 1.00 | 0.00 |
| ATOM | 471 | CA | GLY | S | 445 | 21.400 | 44.330 | 15.159 | 1.00 | 0.00 |
| ATOM | 472 | C | GLY | S | 445 | 20.259 | 44.142 | 14.184 | 1.00 | 0.00 |
| ATOM | 473 | O | GLY | S | 445 | 20.207 | 44.828 | 13.167 | 1.00 | 0.00 |
| ATOM | 474 | H | GLY | S | 445 | 22.293 | 46.074 | 14.285 | 1.00 | 0.00 |
| ATOM | 475 | N | SER | S | 446 | 19.367 | 43.193 | 14.525 | 1.00 | 0.00 |
| ATOM | 476 | CA | SER | S | 446 | 18.306 | 42.770 | 13.600 | 1.00 | 0.00 |
| ATOM | 477 | C | SER | S | 446 | 18.764 | 42.361 | 12.199 | 1.00 | 0.00 |
| ATOM | 478 | O | SER | S | 446 | 19.312 | 43.121 | 11.396 | 1.00 | 0.00 |
| ATOM | 479 | CB | SER | S | 446 | 17.136 | 43.761 | 13.588 | 1.00 | 0.00 |
| ATOM | 480 | OG | SER | S | 446 | 16.580 | 43.870 | 14.909 | 1.00 | 0.00 |
| ATOM | 481 | H | SER | S | 446 | 19.427 | 42.763 | 15.424 | 1.00 | 0.00 |
| ATOM | 482 | HG | SER | S | 446 | 17.085 | 44.577 | 14.294 | 1.00 | 0.00 |
| ATOM | 483 | N | PRO | S | 447 | 18.585 | 41.038 | 11.954 | 1.00 | 0.00 |
| ATOM | 484 | CA | PRO | S | 447 | 19.044 | 40.473 | 10.684 | 1.00 | 0.00 |
| ATOM | 485 | C | PRO | S | 447 | 18.175 | 40.784 | 9.469 | 1.00 | 0.00 |
| ATOM | 486 | O | PRO | S | 447 | 17.544 | 39.906 | 8.891 | 1.00 | 0.00 |
| ATOM | 487 | CB | PRO | S | 447 | 19.119 | 38.978 | 11.018 | 1.00 | 0.00 |
| ATOM | 488 | CG | PRO | S | 447 | 18.005 | 38.753 | 12.042 | 1.00 | 0.00 |
| ATOM | 489 | CD | PRO | S | 447 | 18.035 | 40.036 | 12.862 | 1.00 | 0.00 |
| ATOM | 490 | N | ARG | S | 448 | 18.238 | 42.058 | 9.058 | 1.00 | 0.00 |
| ATOM | 491 | CA | ARG | S | 448 | 17.977 | 42.508 | 7.690 | 1.00 | 0.00 |
| ATOM | 492 | C | ARG | S | 448 | 16.543 | 42.347 | 7.203 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 493 | O | ARG | S | 448 | 16.254 | 41.672 | 6.219 | 1.00 | 0.00 |
| ATOM | 494 | CB | ARG | S | 448 | 18.986 | 41.918 | 6.682 | 1.00 | 0.00 |
| ATOM | 495 | CG | ARG | S | 448 | 20.442 | 41.649 | 7.123 | 1.00 | 0.00 |
| ATOM | 496 | CD | ARG | S | 448 | 21.313 | 42.831 | 7.578 | 1.00 | 0.00 |
| ATOM | 497 | NE | ARG | S | 448 | 21.001 | 43.283 | 8.937 | 1.00 | 0.00 |
| ATOM | 498 | CZ | ARG | S | 448 | 21.531 | 44.422 | 9.424 | 1.00 | 0.00 |
| ATOM | 499 | NH1 | ARG | S | 448 | 21.097 | 44.910 | 10.584 | 1.00 | 0.00 |
| ATOM | 500 | NH2 | ARG | S | 448 | 22.481 | 45.064 | 8.756 | 1.00 | 0.00 |
| ATOM | 501 | H | ARG | S | 448 | 18.359 | 42.706 | 9.806 | 1.00 | 0.00 |
| ATOM | 502 | HE | ARG | S | 448 | 20.335 | 42.788 | 9.500 | 1.00 | 0.00 |
| ATOM | 503 | 1HH1 | ARG | S | 448 | 21.430 | 45.781 | 10.938 | 1.00 | 0.00 |
| ATOM | 504 | 2HH1 | ARG | S | 448 | 20.443 | 44.407 | 11.166 | 1.00 | 0.00 |
| ATOM | 505 | 1HH2 | ARG | S | 448 | 22.741 | 45.988 | 9.014 | 1.00 | 0.00 |
| ATOM | 506 | 2HH2 | ARG | S | 448 | 22.951 | 44.628 | 7.993 | 1.00 | 0.00 |
| ATOM | 507 | N | HIS | S | 449 | 15.650 | 43.000 | 7.953 | 1.00 | 0.00 |
| ATOM | 508 | CA | HIS | S | 449 | 14.277 | 43.153 | 7.487 | 1.00 | 0.00 |
| ATOM | 509 | C | HIS | S | 449 | 13.951 | 44.575 | 7.038 | 1.00 | 0.00 |
| ATOM | 510 | O | HIS | S | 449 | 13.931 | 44.870 | 5.848 | 1.00 | 0.00 |
| ATOM | 511 | CB | HIS | S | 449 | 13.227 | 42.683 | 8.513 | 1.00 | 0.00 |
| ATOM | 512 | CG | HIS | S | 449 | 13.749 | 41.636 | 9.470 | 1.00 | 0.00 |
| ATOM | 513 | ND1 | HIS | S | 449 | 14.569 | 41.937 | 10.493 | 1.00 | 0.00 |
| ATOM | 514 | CD2 | HIS | S | 449 | 13.467 | 40.265 | 9.494 | 1.00 | 0.00 |
| ATOM | 515 | CE1 | HIS | S | 449 | 14.804 | 40.760 | 11.162 | 1.00 | 0.00 |
| ATOM | 516 | NE2 | HIS | S | 449 | 14.129 | 39.735 | 10.554 | 1.00 | 0.00 |
| ATOM | 517 | H | HIS | S | 449 | 15.973 | 43.506 | 8.752 | 1.00 | 0.00 |
| ATOM | 518 | HD1 | HIS | S | 449 | 14.951 | 42.816 | 10.705 | 1.00 | 0.00 |
| ATOM | 519 | N | THR | S | 450 | 13.626 | 45.428 | 8.032 | 1.00 | 0.00 |
| ATOM | 520 | CA | THR | S | 450 | 13.173 | 46.806 | 7.795 | 1.00 | 0.00 |
| ATOM | 521 | C | THR | S | 450 | 12.822 | 47.600 | 9.058 | 1.00 | 0.00 |
| ATOM | 522 | O | THR | S | 450 | 12.599 | 48.805 | 9.018 | 1.00 | 0.00 |
| ATOM | 523 | CB | THR | S | 450 | 12.013 | 46.862 | 6.757 | 1.00 | 0.00 |
| ATOM | 524 | OG1 | THR | S | 450 | 11.743 | 48.196 | 6.306 | 1.00 | 0.00 |
| ATOM | 525 | CG2 | THR | S | 450 | 10.730 | 46.190 | 7.255 | 1.00 | 0.00 |
| ATOM | 526 | H | THR | S | 450 | 13.888 | 45.118 | 8.945 | 1.00 | 0.00 |
| ATOM | 527 | HG1 | THR | S | 450 | 12.483 | 48.478 | 5.767 | 1.00 | 0.00 |
| ATOM | 528 | N | VAL | S | 451 | 12.696 | 46.895 | 10.195 | 1.00 | 0.00 |
| ATOM | 529 | CA | VAL | S | 451 | 12.153 | 47.702 | 11.287 | 1.00 | 0.00 |
| ATOM | 530 | C | VAL | S | 451 | 13.179 | 48.295 | 12.260 | 1.00 | 0.00 |
| ATOM | 531 | O | VAL | S | 451 | 13.427 | 49.500 | 12.206 | 1.00 | 0.00 |
| ATOM | 532 | CB | VAL | S | 451 | 10.914 | 47.060 | 11.957 | 1.00 | 0.00 |
| ATOM | 533 | CG1 | VAL | S | 451 | 10.097 | 48.103 | 12.721 | 1.00 | 0.00 |
| ATOM | 534 | CG2 | VAL | S | 451 | 10.037 | 46.294 | 10.965 | 1.00 | 0.00 |
| ATOM | 535 | H | VAL | S | 451 | 13.116 | 45.993 | 10.321 | 1.00 | 0.00 |
| ATOM | 536 | N | PRO | S | 452 | 13.782 | 47.463 | 13.160 | 1.00 | 0.00 |
| ATOM | 537 | CA | PRO | S | 452 | 14.742 | 48.047 | 14.097 | 1.00 | 0.00 |
| ATOM | 538 | C | PRO | S | 452 | 16.079 | 48.335 | 13.439 | 1.00 | 0.00 |
| ATOM | 539 | O | PRO | S | 452 | 17.018 | 47.548 | 13.514 | 1.00 | 0.00 |
| ATOM | 540 | CB | PRO | S | 452 | 14.871 | 46.982 | 15.196 | 1.00 | 0.00 |
| ATOM | 541 | CG | PRO | S | 452 | 13.816 | 45.915 | 14.903 | 1.00 | 0.00 |
| ATOM | 542 | CD | PRO | S | 452 | 13.629 | 46.032 | 13.399 | 1.00 | 0.00 |
| ATOM | 543 | N | GLN | S | 453 | 16.120 | 49.513 | 12.808 | 1.00 | 0.00 |
| ATOM | 544 | CA | GLN | S | 453 | 17.317 | 49.925 | 12.082 | 1.00 | 0.00 |
| ATOM | 545 | C | GLN | S | 453 | 18.587 | 49.982 | 12.900 | 1.00 | 0.00 |
| ATOM | 546 | O | GLN | S | 453 | 18.581 | 50.139 | 14.121 | 1.00 | 0.00 |
| ATOM | 547 | CB | GLN | S | 453 | 17.038 | 51.254 | 11.420 | 1.00 | 0.00 |
| ATOM | 548 | CG | GLN | S | 453 | 15.926 | 51.091 | 10.389 | 1.00 | 0.00 |
| ATOM | 549 | CD | GLN | S | 453 | 15.375 | 52.450 | 10.056 | 1.00 | 0.00 |
| ATOM | 550 | OE1 | GLN | S | 453 | 14.170 | 52.689 | 10.072 | 1.00 | 0.00 |
| ATOM | 551 | NE2 | GLN | S | 453 | 16.305 | 53.354 | 9.751 | 1.00 | 0.00 |
| ATOM | 552 | H | GLN | S | 453 | 15.279 | 50.052 | 12.766 | 1.00 | 0.00 |
| ATOM | 553 | 1HE2 | GLN | S | 453 | 16.031 | 54.296 | 9.570 | 1.00 | 0.00 |
| ATOM | 554 | 2HE2 | GLN | S | 453 | 17.275 | 53.095 | 9.744 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 555 | N | CYS | S | 454 | 19.674 | 49.781 | 12.143 | 1.00 | 0.00 |
| ATOM | 556 | CA | CYS | S | 454 | 20.979 | 49.500 | 12.752 | 1.00 | 0.00 |
| ATOM | 557 | C | CYS | S | 454 | 21.470 | 50.622 | 13.657 | 1.00 | 0.00 |
| ATOM | 558 | O | CYS | S | 454 | 20.971 | 51.743 | 13.611 | 1.00 | 0.00 |
| ATOM | 559 | CB | CYS | S | 454 | 22.006 | 49.226 | 11.657 | 1.00 | 0.00 |
| ATOM | 560 | SG | CYS | S | 454 | 21.338 | 48.159 | 10.350 | 1.00 | 0.00 |
| ATOM | 561 | H | CYS | S | 454 | 19.490 | 49.752 | 11.162 | 1.00 | 0.00 |
| ATOM | 562 | N | CYS | S | 455 | 22.482 | 50.313 | 14.491 | 1.00 | 0.00 |
| ATOM | 563 | CA | CYS | S | 455 | 22.980 | 51.419 | 15.325 | 1.00 | 0.00 |
| ATOM | 564 | C | CYS | S | 455 | 23.755 | 52.455 | 14.521 | 1.00 | 0.00 |
| ATOM | 565 | O | CYS | S | 455 | 24.018 | 52.227 | 13.336 | 1.00 | 0.00 |
| ATOM | 566 | CB | CYS | S | 455 | 23.853 | 50.894 | 16.460 | 1.00 | 0.00 |
| ATOM | 567 | SG | CYS | S | 455 | 23.196 | 49.448 | 17.341 | 1.00 | 0.00 |
| ATOM | 568 | H | CYS | S | 455 | 22.933 | 49.419 | 14.477 | 1.00 | 0.00 |
| ATOM | 569 | N | TYR | S | 456 | 24.119 | 53.580 | 15.183 | 1.00 | 0.00 |
| ATOM | 570 | CA | TYR | S | 456 | 24.860 | 54.653 | 14.502 | 1.00 | 0.00 |
| ATOM | 571 | C | TYR | S | 456 | 25.450 | 55.690 | 15.461 | 1.00 | 0.00 |
| ATOM | 572 | O | TYR | S | 456 | 25.005 | 55.852 | 16.594 | 1.00 | 0.00 |
| ATOM | 573 | CB | TYR | S | 456 | 23.899 | 55.315 | 13.507 | 1.00 | 0.00 |
| ATOM | 574 | CG | TYR | S | 456 | 24.487 | 56.450 | 12.704 | 1.00 | 0.00 |
| ATOM | 575 | CD1 | TYR | S | 456 | 25.356 | 56.181 | 11.631 | 1.00 | 0.00 |
| ATOM | 576 | CD2 | TYR | S | 456 | 24.116 | 57.761 | 13.052 | 1.00 | 0.00 |
| ATOM | 577 | CE1 | TYR | S | 456 | 25.806 | 57.260 | 10.854 | 1.00 | 0.00 |
| ATOM | 578 | CE2 | TYR | S | 456 | 24.564 | 58.837 | 12.273 | 1.00 | 0.00 |
| ATOM | 579 | CZ | TYR | S | 456 | 25.376 | 58.569 | 11.158 | 1.00 | 0.00 |
| ATOM | 580 | OH | TYR | S | 456 | 25.732 | 59.625 | 10.345 | 1.00 | 0.00 |
| ATOM | 581 | H | TYR | S | 456 | 23.682 | 53.782 | 16.058 | 1.00 | 0.00 |
| ATOM | 582 | HH | TYR | S | 456 | 26.667 | 59.534 | 10.136 | 1.00 | 0.00 |
| ATOM | 583 | N | GLY | S | 457 | 26.441 | 56.452 | 14.956 | 1.00 | 0.00 |
| ATOM | 584 | CA | GLY | S | 457 | 26.709 | 57.754 | 15.567 | 1.00 | 0.00 |
| ATOM | 585 | C | GLY | S | 457 | 27.578 | 58.605 | 14.667 | 1.00 | 0.00 |
| ATOM | 586 | O | GLY | S | 457 | 28.272 | 58.076 | 13.811 | 1.00 | 0.00 |
| ATOM | 587 | H | GLY | S | 457 | 26.963 | 56.179 | 14.140 | 1.00 | 0.00 |
| ATOM | 588 | N | PHE | S | 458 | 27.571 | 59.917 | 14.923 | 1.00 | 0.00 |
| ATOM | 589 | CA | PHE | S | 458 | 28.646 | 60.677 | 14.289 | 1.00 | 0.00 |
| ATOM | 590 | C | PHE | S | 458 | 30.015 | 60.446 | 14.912 | 1.00 | 0.00 |
| ATOM | 591 | O | PHE | S | 458 | 31.054 | 60.812 | 14.368 | 1.00 | 0.00 |
| ATOM | 592 | CB | PHE | S | 458 | 28.295 | 62.162 | 14.232 | 1.00 | 0.00 |
| ATOM | 593 | CG | PHE | S | 458 | 27.073 | 62.351 | 13.363 | 1.00 | 0.00 |
| ATOM | 594 | CD1 | PHE | S | 458 | 25.796 | 62.428 | 13.936 | 1.00 | 0.00 |
| ATOM | 595 | CD2 | PHE | S | 458 | 27.231 | 62.450 | 11.963 | 1.00 | 0.00 |
| ATOM | 596 | CE1 | PHE | S | 458 | 24.660 | 62.606 | 13.150 | 1.00 | 0.00 |
| ATOM | 597 | CE2 | PHE | S | 458 | 26.096 | 62.630 | 11.150 | 1.00 | 0.00 |
| ATOM | 598 | CZ | PHE | S | 458 | 24.822 | 62.705 | 11.752 | 1.00 | 0.00 |
| ATOM | 599 | H | PHE | S | 458 | 26.988 | 60.332 | 15.619 | 1.00 | 0.00 |
| ATOM | 600 | N | CYS | S | 459 | 29.996 | 59.778 | 16.079 | 1.00 | 0.00 |
| ATOM | 601 | CA | CYS | S | 459 | 31.253 | 59.146 | 16.496 | 1.00 | 0.00 |
| ATOM | 602 | C | CYS | S | 459 | 31.778 | 59.109 | 15.512 | 1.00 | 0.00 |
| ATOM | 603 | O | CYS | S | 459 | 32.972 | 57.854 | 15.395 | 1.00 | 0.00 |
| ATOM | 604 | CB | CYS | S | 459 | 31.122 | 58.494 | 17.867 | 1.00 | 0.00 |
| ATOM | 605 | SG | CYS | S | 459 | 30.818 | 59.692 | 19.192 | 1.00 | 0.00 |
| ATOM | 606 | H | CYS | S | 459 | 29.115 | 59.528 | 16.467 | 1.00 | 0.00 |
| ATOM | 607 | N | ILE | S | 460 | 30.830 | 57.504 | 14.786 | 1.00 | 0.00 |
| ATOM | 608 | CA | ILE | S | 460 | 31.293 | 56.464 | 13.872 | 1.00 | 0.00 |
| ATOM | 609 | C | ILE | S | 460 | 31.537 | 56.972 | 12.453 | 1.00 | 0.00 |
| ATOM | 610 | O | ILE | S | 460 | 32.377 | 56.452 | 11.705 | 1.00 | 0.00 |
| ATOM | 611 | CB | ILE | S | 460 | 30.382 | 55.231 | 13.940 | 1.00 | 0.00 |
| ATOM | 612 | CG1 | ILE | S | 460 | 29.950 | 54.935 | 15.387 | 1.00 | 0.00 |
| ATOM | 613 | CG2 | ILE | S | 460 | 31.117 | 54.021 | 13.356 | 1.00 | 0.00 |
| ATOM | 614 | CD1 | ILE | S | 460 | 31.088 | 54.488 | 16.317 | 1.00 | 0.00 |
| ATOM | 615 | H | ILE | S | 460 | 29.925 | 57.914 | 14.690 | 1.00 | 0.00 |
| ATOM | 616 | N | ASP | S | 461 | 30.869 | 58.108 | 12.169 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 617 | CA | ASP | S | 461 | 31.370 | 58.928 | 11.064 | 1.00 | 0.00 |
| ATOM | 618 | C | ASP | S | 461 | 32.714 | 59.562 | 11.410 | 1.00 | 0.00 |
| ATOM | 619 | O | ASP | S | 461 | 33.602 | 59.761 | 10.584 | 1.00 | 0.00 |
| ATOM | 620 | CB | ASP | S | 461 | 30.316 | 59.933 | 10.557 | 1.00 | 0.00 |
| ATOM | 621 | CG | ASP | S | 461 | 29.111 | 59.192 | 9.986 | 1.00 | 0.00 |
| ATOM | 622 | OD1 | ASP | S | 461 | 28.443 | 58.818 | 10.754 | 1.00 | 0.00 |
| ATOM | 623 | OD2 | ASP | S | 461 | 28.819 | 59.257 | 8.789 | 1.00 | 0.00 |
| ATOM | 624 | H | ASP | S | 461 | 30.045 | 58.376 | 12.672 | 1.00 | 0.00 |
| ATOM | 625 | N | LEU | S | 462 | 32.932 | 59.714 | 12.731 | 1.00 | 0.00 |
| ATOM | 626 | CA | LEU | S | 462 | 34.315 | 59.947 | 13.165 | 1.00 | 0.00 |
| ATOM | 627 | C | LEU | S | 462 | 35.288 | 58.823 | 12.831 | 1.00 | 0.00 |
| ATOM | 628 | O | LEU | S | 462 | 36.497 | 59.032 | 12.804 | 1.00 | 0.00 |
| ATOM | 629 | CB | LEU | S | 462 | 34.445 | 60.338 | 14.640 | 1.00 | 0.00 |
| ATOM | 630 | CG | LEU | S | 462 | 35.148 | 61.665 | 14.945 | 1.00 | 0.00 |
| ATOM | 631 | CD1 | LEU | S | 462 | 35.412 | 61.781 | 16.444 | 1.00 | 0.00 |
| ATOM | 632 | CD2 | LEU | S | 462 | 26.421 | 61.908 | 14.131 | 1.00 | 0.00 |
| ATOM | 633 | H | LEU | S | 462 | 32.162 | 59.694 | 13.366 | 1.00 | 0.00 |
| ATOM | 634 | N | LEU | S | 463 | 34.747 | 57.657 | 12.473 | 1.00 | 0.00 |
| ATOM | 635 | CA | LEU | S | 463 | 35.577 | 56.668 | 11.786 | 1.00 | 0.00 |
| ATOM | 636 | C | LEU | S | 463 | 35.742 | 56.840 | 10.281 | 1.00 | 0.00 |
| ATOM | 637 | O | LEU | S | 463 | 36.661 | 56.275 | 9.701 | 1.00 | 0.00 |
| ATOM | 638 | CB | LEU | S | 463 | 35.160 | 55.228 | 12.096 | 1.00 | 0.00 |
| ATOM | 639 | CG | LEU | S | 463 | 35.174 | 54.883 | 13.584 | 1.00 | 0.00 |
| ATOM | 640 | CD1 | LEU | S | 463 | 34.710 | 53.448 | 13.827 | 1.00 | 0.00 |
| ATOM | 641 | CD2 | LEU | S | 463 | 36.538 | 55.143 | 14.215 | 1.00 | 0.00 |
| ATOM | 642 | H | LEU | S | 463 | 33.768 | 57.557 | 12.611 | 1.00 | 0.00 |
| ATOM | 643 | N | ILE | S | 464 | 34.926 | 57.682 | 9.633 | 1.00 | 0.00 |
| ATOM | 644 | CA | ILE | S | 464 | 35.205 | 57.975 | 8.211 | 1.00 | 0.00 |
| ATOM | 645 | C | ILE | S | 464 | 36.656 | 58.351 | 7.906 | 1.00 | 0.00 |
| ATOM | 646 | O | ILE | S | 464 | 37.348 | 57.555 | 7.154 | 1.00 | 0.00 |
| ATOM | 647 | CB | ILE | S | 464 | 34.236 | 59.016 | 7.612 | 1.00 | 0.00 |
| ATOM | 648 | CG1 | ILE | S | 464 | 32.807 | 58.479 | 7.669 | 1.00 | 0.00 |
| ATOM | 649 | CG2 | ILE | S | 464 | 34.592 | 59.360 | 6.156 | 1.00 | 0.00 |
| ATOM | 650 | CD1 | ILE | S | 464 | 31.775 | 59.409 | 7.027 | 1.00 | 0.00 |
| ATOM | 651 | H | ILE | S | 464 | 34.079 | 57.977 | 10.069 | 1.00 | 0.00 |
| ATOM | 652 | N | LYS | S | 465 | 37.128 | 59.425 | 8.557 | 1.00 | 0.00 |
| ATOM | 653 | CA | LYS | S | 465 | 38.535 | 59.777 | 8.344 | 1.00 | 0.00 |
| ATOM | 654 | C | LYS | S | 465 | 39.601 | 58.763 | 8.741 | 1.00 | 0.00 |
| ATOM | 655 | O | LYS | S | 465 | 40.778 | 58.981 | 8.469 | 1.00 | 0.00 |
| ATOM | 656 | CB | LYS | S | 465 | 38.894 | 61.103 | 9.003 | 1.00 | 0.00 |
| ATOM | 657 | CG | LYS | S | 465 | 38.574 | 62.312 | 8.131 | 1.00 | 0.00 |
| ATOM | 658 | CD | LYS | S | 465 | 39.289 | 63.544 | 8.671 | 1.00 | 0.00 |
| ATOM | 659 | CE | LYS | S | 465 | 38.974 | 64.823 | 7.905 | 1.00 | 0.00 |
| ATOM | 660 | NZ | LYS | S | 465 | 39.913 | 65.868 | 8.325 | 1.00 | 0.00 |
| ATOM | 661 | H | LYS | S | 465 | 36.513 | 60.049 | 9.031 | 1.00 | 0.00 |
| ATOM | 662 | 1HZ | LYS | S | 465 | 40.495 | 66.073 | 7.489 | 1.00 | 0.00 |
| ATOM | 663 | 2HZ | LYS | S | 465 | 39.401 | 66.718 | 8.646 | 1.00 | 0.00 |
| ATOM | 664 | 3HZ | LYS | S | 465 | 40.548 | 65.557 | 9.089 | 1.00 | 0.00 |
| ATOM | 665 | N | LEU | S | 466 | 39.156 | 57.684 | 9.402 | 1.00 | 0.00 |
| ATOM | 666 | CA | LEU | S | 466 | 40.119 | 56.695 | 9.882 | 1.00 | 0.00 |
| ATOM | 667 | C | LEU | S | 466 | 39.985 | 55.355 | 9.166 | 1.00 | 0.00 |
| ATOM | 668 | O | LEU | S | 466 | 40.857 | 54.877 | 8.432 | 1.00 | 0.00 |
| ATOM | 669 | CB | LEU | S | 466 | 39.985 | 56.514 | 11.404 | 1.00 | 0.00 |
| ATOM | 670 | CG | LEU | S | 466 | 39.762 | 57.797 | 12.223 | 1.00 | 0.00 |
| ATOM | 671 | CD1 | LEU | S | 466 | 39.515 | 57.485 | 13.699 | 1.00 | 0.00 |
| ATOM | 672 | CD2 | LEU | S | 466 | 40.881 | 58.825 | 12.065 | 1.00 | 0.00 |
| ATOM | 673 | H | LEU | S | 466 | 38.181 | 57.575 | 9.578 | 1.00 | 0.00 |
| ATOM | 674 | N | ALA | S | 467 | 38.812 | 54.730 | 9.383 | 1.00 | 0.00 |
| ATOM | 675 | CA | ALA | S | 467 | 38.497 | 53.429 | 8.792 | 1.00 | 0.00 |
| ATOM | 676 | C | ALA | S | 467 | 38.572 | 53.382 | 7.278 | 1.00 | 0.00 |
| ATOM | 677 | O | ALA | S | 467 | 39.069 | 52.427 | 6.691 | 1.00 | 0.00 |
| ATOM | 678 | CB | ALA | S | 467 | 37.106 | 52.963 | 9.224 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 679 | H | ALA | S | 467 | 38.160 | 55.164 | 10.005 | 1.00 | 0.00 |
| ATOM | 680 | N | ARG | S | 468 | 38.107 | 54.473 | 6.652 | 1.00 | 0.00 |
| ATOM | 681 | CA | ARG | S | 468 | 38.128 | 54.507 | 5.183 | 1.00 | 0.00 |
| ATOM | 682 | C | ARG | S | 468 | 39.479 | 54.922 | 4.586 | 1.00 | 0.00 |
| ATOM | 683 | O | ARG | S | 468 | 39.571 | 55.627 | 3.584 | 1.00 | 0.00 |
| ATOM | 684 | CB | ARG | S | 468 | 36.946 | 55.352 | 4.669 | 1.00 | 0.00 |
| ATOM | 685 | CG | ARG | S | 468 | 35.572 | 54.038 | 5.238 | 1.00 | 0.00 |
| ATOM | 686 | CD | ARG | S | 468 | 34.388 | 55.740 | 4.664 | 1.00 | 0.00 |
| ATOM | 687 | NE | ARG | S | 468 | 33.109 | 55.401 | 5.308 | 1.00 | 0.00 |
| ATOM | 688 | CZ | ARG | S | 468 | 31.995 | 56.166 | 5.145 | 1.00 | 0.00 |
| ATOM | 689 | NH1 | ARG | S | 468 | 30.874 | 55.865 | 5.796 | 1.00 | 0.00 |
| ATOM | 690 | NH2 | ARG | S | 468 | 32.020 | 57.227 | 4.351 | 1.00 | 0.00 |
| ATOM | 691 | H | ARG | S | 468 | 37.842 | 55.290 | 7.165 | 1.00 | 0.00 |
| ATOM | 692 | HE | ARG | S | 468 | 33.089 | 54.649 | 5.976 | 1.00 | 0.00 |
| ATOM | 693 | 1HH1 | ARG | S | 468 | 30.064 | 56.464 | 5.783 | 1.00 | 0.00 |
| ATOM | 694 | 2HH1 | ARG | S | 468 | 30.809 | 55.036 | 6.361 | 1.00 | 0.00 |
| ATOM | 695 | 1HH2 | ARG | S | 468 | 31.256 | 57.872 | 4.329 | 1.00 | 0.00 |
| ATOM | 696 | 2HH2 | ARG | S | 468 | 32.817 | 57.397 | 3.777 | 1.00 | 0.00 |
| ATOM | 697 | N | THR | S | 469 | 40.526 | 54.431 | 5.277 | 1.00 | 0.00 |
| ATOM | 698 | CA | THR | S | 469 | 41.926 | 54.770 | 5.042 | 1.00 | 0.00 |
| ATOM | 699 | C | THR | S | 469 | 42.869 | 53.643 | 5.477 | 1.00 | 0.00 |
| ATOM | 700 | O | THR | S | 469 | 43.738 | 53.207 | 4.729 | 1.00 | 0.00 |
| ATOM | 701 | CB | THR | S | 469 | 42.290 | 56.065 | 5.792 | 1.00 | 0.00 |
| ATOM | 702 | OG1 | THR | S | 469 | 41.178 | 56.974 | 5.844 | 1.00 | 0.00 |
| ATOM | 703 | CG2 | THR | S | 469 | 43.526 | 56.744 | 8.201 | 1.00 | 0.00 |
| ATOM | 704 | H | THR | S | 469 | 40.306 | 53.779 | 5.994 | 1.00 | 0.00 |
| ATOM | 705 | HG1 | THR | S | 469 | 40.583 | 56.624 | 6.510 | 1.00 | 0.00 |
| ATOM | 706 | N | MET | S | 470 | 42.652 | 53.208 | 6.750 | 1.00 | 0.00 |
| ATOM | 707 | CA | MET | S | 470 | 43.650 | 52.414 | 7.493 | 1.00 | 0.00 |
| ATOM | 708 | C | MET | S | 470 | 44.471 | 51.444 | 6.669 | 1.00 | 0.00 |
| ATOM | 709 | O | MET | S | 470 | 45.689 | 51.547 | 6.570 | 1.00 | 0.00 |
| ATOM | 710 | CB | MET | S | 470 | 43.044 | 51.690 | 8.704 | 1.00 | 0.00 |
| ATOM | 711 | CG | MET | S | 470 | 42.788 | 52.603 | 9.907 | 1.00 | 0.00 |
| ATOM | 712 | SD | MET | S | 470 | 42.311 | 51.692 | 11.387 | 1.00 | 0.00 |
| ATOM | 713 | CE | MET | S | 470 | 41.945 | 53.100 | 12.447 | 1.00 | 0.00 |
| ATOM | 714 | H | MET | S | 470 | 41.819 | 53.492 | 7.220 | 1.00 | 0.00 |
| ATOM | 715 | N | ASN | S | 471 | 43.736 | 50.557 | 5.992 | 1.00 | 0.00 |
| ATOM | 716 | CA | ASN | S | 471 | 44.370 | 50.007 | 4.801 | 1.00 | 0.00 |
| ATOM | 717 | C | ASN | S | 471 | 43.434 | 50.128 | 3.630 | 1.00 | 0.00 |
| ATOM | 718 | O | ASN | S | 471 | 42.247 | 49.825 | 3.714 | 1.00 | 0.00 |
| ATOM | 719 | CB | ASN | S | 471 | 44.799 | 48.553 | 4.977 | 1.00 | 0.00 |
| ATOM | 720 | CG | ASN | S | 471 | 46.143 | 48.479 | 5.661 | 1.00 | 0.00 |
| ATOM | 721 | OD1 | ASN | S | 471 | 47.158 | 48.936 | 5.151 | 1.00 | 0.00 |
| ATOM | 722 | ND2 | ASN | S | 471 | 46.137 | 47.838 | 6.821 | 1.00 | 0.00 |
| ATOM | 723 | H | ASN | S | 471 | 42.750 | 50.483 | 6.142 | 1.00 | 0.00 |
| ATOM | 724 | 1HD2 | ASN | S | 471 | 46.978 | 47.679 | 7.322 | 1.00 | 0.00 |
| ATOM | 725 | 2HD2 | ASN | S | 471 | 45.279 | 47.576 | 7.273 | 1.00 | 0.00 |
| ATOM | 726 | N | PHE | S | 472 | 44.024 | 50.572 | 2.512 | 1.00 | 0.00 |
| ATOM | 727 | CA | PHE | S | 472 | 43.264 | 50.597 | 1.257 | 1.00 | 0.00 |
| ATOM | 728 | C | PHE | S | 472 | 42.933 | 49.216 | 0.705 | 1.00 | 0.00 |
| ATOM | 729 | O | PHE | S | 472 | 42.035 | 49.013 | -0.102 | 1.00 | 0.00 |
| ATOM | 730 | CB | PHE | S | 472 | 43.976 | 51.471 | 0.221 | 1.00 | 0.00 |
| ATOM | 731 | CG | PHE | S | 472 | 44.093 | 52.884 | 0.750 | 1.00 | 0.00 |
| ATOM | 732 | CD1 | PHE | S | 472 | 45.341 | 53.345 | 1.224 | 1.00 | 0.00 |
| ATOM | 733 | CD2 | PHE | S | 472 | 42.952 | 53.717 | 0.771 | 1.00 | 0.00 |
| ATOM | 734 | CE1 | PHE | S | 472 | 45.449 | 54.654 | 1.733 | 1.00 | 0.00 |
| ATOM | 735 | CE2 | PHE | S | 472 | 43.058 | 55.026 | 1.279 | 1.00 | 0.00 |
| ATOM | 736 | CZ | PHE | S | 472 | 44.305 | 55.480 | 1.756 | 1.00 | 0.00 |
| ATOM | 737 | H | PHE | S | 472 | 44.965 | 50.914 | 2.566 | 1.00 | 0.00 |
| ATOM | 738 | N | THR | S | 473 | 43.660 | 48.230 | 1.255 | 1.00 | 0.00 |
| ATOM | 739 | CA | THR | S | 473 | 43.158 | 46.873 | 1.087 | 1.00 | 0.00 |
| ATOM | 740 | C | THR | S | 473 | 42.016 | 46.545 | 2.056 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 741 | O | THR | S | 473 | 42.103 | 45.714 | 2.957 | 1.00 | 0.00 |
| ATOM | 742 | CB | THR | S | 473 | 44.338 | 45.880 | 1.116 | 1.00 | 0.00 |
| ATOM | 743 | OG1 | THR | S | 473 | 43.915 | 44.559 | 0.775 | 1.00 | 0.00 |
| ATOM | 744 | CG2 | THR | S | 473 | 45.147 | 45.887 | 2.416 | 1.00 | 0.00 |
| ATOM | 745 | H | THR | S | 473 | 44.363 | 48.459 | 1.921 | 1.00 | 0.00 |
| ATOM | 746 | HG1 | THR | S | 473 | 43.298 | 44.303 | 1.453 | 1.00 | 0.00 |
| ATOM | 747 | N | TYR | S | 474 | 40.904 | 47.249 | 1.802 | 1.00 | 0.00 |
| ATOM | 748 | CA | TYR | S | 474 | 39.624 | 46.979 | 2.449 | 1.00 | 0.00 |
| ATOM | 749 | C | TYR | S | 474 | 39.555 | 47.140 | 3.964 | 1.00 | 0.00 |
| ATOM | 750 | O | TYR | S | 474 | 38.558 | 46.760 | 4.576 | 1.00 | 0.00 |
| ATOM | 751 | CB | TYR | S | 474 | 39.042 | 45.606 | 2.041 | 1.00 | 0.00 |
| ATOM | 752 | CG | TYR | S | 474 | 39.219 | 45.297 | 0.565 | 1.00 | 0.00 |
| ATOM | 753 | CD1 | TYR | S | 474 | 40.253 | 44.417 | 0.183 | 1.00 | 0.00 |
| ATOM | 754 | CD2 | TYR | S | 474 | 38.354 | 45.876 | -0.389 | 1.00 | 0.00 |
| ATOM | 755 | CE1 | TYR | S | 474 | 40.435 | 44.117 | -1.177 | 1.00 | 0.00 |
| ATOM | 756 | CE2 | TYR | S | 474 | 38.530 | 45.567 | -1.751 | 1.00 | 0.00 |
| ATOM | 757 | CZ | TYR | S | 474 | 39.573 | 44.696 | -2.130 | 1.00 | 0.00 |
| ATOM | 758 | OH | TYR | S | 474 | 39.772 | 44.399 | -3.468 | 1.00 | 0.00 |
| ATOM | 759 | H | TYR | S | 474 | 40.949 | 47.933 | 1.074 | 1.00 | 0.00 |
| ATOM | 760 | HH | TYR | S | 474 | 40.714 | 44.379 | -3.591 | 1.00 | 0.00 |
| ATOM | 761 | N | GLU | S | 475 | 40.599 | 47.712 | 4.587 | 1.00 | 0.00 |
| ATOM | 762 | CA | GLU | S | 475 | 40.574 | 47.703 | 6.053 | 1.00 | 0.00 |
| ATOM | 763 | C | GLU | S | 475 | 39.794 | 48.808 | 6.757 | 1.00 | 0.00 |
| ATOM | 764 | O | GLU | S | 475 | 40.215 | 49.425 | 7.734 | 1.00 | 0.00 |
| ATOM | 765 | CB | GLU | S | 475 | 41.962 | 47.480 | 6.660 | 1.00 | 0.00 |
| ATOM | 766 | CG | GLU | S | 475 | 41.940 | 46.853 | 8.061 | 1.00 | 0.00 |
| ATOM | 767 | CD | GLU | S | 475 | 43.338 | 46.769 | 8.644 | 1.00 | 0.00 |
| ATOM | 768 | OE1 | GLU | S | 475 | 43.981 | 47.811 | 8.788 | 1.00 | 0.00 |
| ATOM | 769 | OE2 | GLU | S | 475 | 43.779 | 45.663 | 8.966 | 1.00 | 0.00 |
| ATOM | 770 | H | GLU | S | 475 | 41.365 | 48.095 | 4.068 | 1.00 | 0.00 |
| ATOM | 771 | N | VAL | S | 476 | 38.561 | 48.962 | 6.255 | 1.00 | 0.00 |
| ATOM | 772 | CA | VAL | S | 476 | 37.514 | 49.475 | 7.133 | 1.00 | 0.00 |
| ATOM | 773 | C | VAL | S | 476 | 37.283 | 48.569 | 8.341 | 1.00 | 0.00 |
| ATOM | 774 | O | VAL | S | 476 | 37.877 | 47.495 | 8.491 | 1.00 | 0.00 |
| ATOM | 775 | CB | VAL | S | 476 | 36.214 | 49.698 | 6.343 | 1.00 | 0.00 |
| ATOM | 776 | CG1 | VAL | S | 476 | 36.414 | 50.771 | 5.270 | 1.00 | 0.00 |
| ATOM | 777 | CG2 | VAL | S | 476 | 35.654 | 48.396 | 5.757 | 1.00 | 0.00 |
| ATOM | 778 | H | VAL | S | 476 | 38.304 | 48.507 | 5.407 | 1.00 | 0.00 |
| ATOM | 779 | N | HIS | S | 477 | 36.414 | 49.072 | 9.221 | 1.00 | 0.00 |
| ATOM | 780 | CA | HIS | S | 477 | 36.089 | 48.258 | 10.382 | 1.00 | 0.00 |
| ATOM | 781 | C | HIS | S | 477 | 35.062 | 47.182 | 10.101 | 1.00 | 0.00 |
| ATOM | 782 | O | HIS | S | 477 | 34.417 | 47.085 | 9.060 | 1.00 | 0.00 |
| ATOM | 783 | CB | HIS | S | 477 | 35.653 | 49.131 | 11.563 | 1.00 | 0.00 |
| ATOM | 784 | CG | HIS | S | 477 | 36.873 | 49.738 | 12.211 | 1.00 | 0.00 |
| ATOM | 785 | ND1 | HIS | S | 477 | 37.943 | 49.023 | 12.603 | 1.00 | 0.00 |
| ATOM | 786 | CD2 | HIS | S | 477 | 37.108 | 51.084 | 12.503 | 1.00 | 0.00 |
| ATOM | 787 | CE1 | HIS | S | 477 | 38.875 | 49.900 | 13.132 | 1.00 | 0.00 |
| ATOM | 788 | NE2 | HIS | S | 477 | 30.337 | 51.172 | 13.073 | 1.00 | 0.00 |
| ATOM | 789 | H | HIS | S | 477 | 35.814 | 49.820 | 8.950 | 1.00 | 0.00 |
| ATOM | 790 | HD1 | HIS | S | 477 | 38.065 | 48.049 | 12.576 | 1.00 | 0.00 |
| ATOM | 791 | N | LEU | S | 478 | 34.934 | 46.330 | 11.122 | 1.00 | 0.00 |
| ATOM | 792 | CA | LEU | S | 478 | 33.935 | 45.269 | 11.085 | 1.00 | 0.00 |
| ATOM | 793 | C | LEU | S | 478 | 33.343 | 45.091 | 12.468 | 1.00 | 0.00 |
| ATOM | 794 | O | LEU | S | 478 | 33.764 | 45.704 | 13.449 | 1.00 | 0.00 |
| ATOM | 795 | CB | LEU | S | 478 | 34.551 | 43.964 | 10.570 | 1.00 | 0.00 |
| ATOM | 796 | CG | LEU | S | 478 | 33.560 | 43.015 | 9.883 | 1.00 | 0.00 |
| ATOM | 797 | CD1 | LEU | S | 478 | 32.998 | 43.613 | 8.592 | 1.00 | 0.00 |
| ATOM | 798 | CD2 | LEU | S | 478 | 34.141 | 41.616 | 9.679 | 1.00 | 0.00 |
| ATOM | 799 | H | LEU | S | 478 | 35.360 | 46.496 | 12.015 | 1.00 | 0.00 |
| ATOM | 800 | N | VAL | S | 479 | 32.314 | 44.233 | 12.526 | 1.00 | 0.00 |
| ATOM | 801 | CA | VAL | S | 479 | 31.576 | 43.932 | 13.754 | 1.00 | 0.00 |
| ATOM | 802 | C | VAL | S | 479 | 30.555 | 42.877 | 13.384 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 803 | O | VAL | S | 479 | 30.092 | 42.879 | 12.249 | 1.00 | 0.00 |
| ATOM | 804 | CB | VAL | S | 479 | 30.893 | 45.210 | 14.293 | 1.00 | 0.00 |
| ATOM | 805 | CG1 | VAL | S | 479 | 30.019 | 45.863 | 13.220 | 1.00 | 0.00 |
| ATOM | 806 | CG2 | VAL | S | 479 | 30.170 | 45.014 | 15.361 | 1.00 | 0.00 |
| ATOM | 807 | H | VAL | S | 479 | 31.991 | 43.836 | 11.664 | 1.00 | 0.00 |
| ATOM | 808 | N | ALA | S | 480 | 30.211 | 42.011 | 14.349 | 1.00 | 0.00 |
| ATOM | 809 | CA | ALA | S | 480 | 29.016 | 41.196 | 14.125 | 1.00 | 0.00 |
| ATOM | 810 | C | ALA | S | 480 | 27.835 | 41.968 | 14.703 | 1.00 | 0.00 |
| ATOM | 811 | O | ALA | S | 480 | 27.719 | 43.173 | 14.449 | 1.00 | 0.00 |
| ATOM | 812 | CB | ALA | S | 480 | 29.219 | 39.817 | 14.766 | 1.00 | 0.00 |
| ATOM | 813 | H | ALA | S | 480 | 30.572 | 42.130 | 15.273 | 1.00 | 0.00 |
| ATOM | 814 | N | ASP | S | 481 | 27.010 | 41.310 | 15.536 | 1.00 | 0.00 |
| ATOM | 815 | CA | ASP | S | 481 | 26.420 | 42.066 | 16.642 | 1.00 | 0.00 |
| ATOM | 816 | C | ASP | S | 481 | 27.524 | 42.608 | 17.552 | 1.00 | 0.00 |
| ATOM | 817 | O | ASP | S | 481 | 28.708 | 42.294 | 17.373 | 1.00 | 0.00 |
| ATOM | 818 | CB | ASP | S | 481 | 25.486 | 41.143 | 17.446 | 1.00 | 0.00 |
| ATOM | 819 | CG | ASP | S | 481 | 26.310 | 40.163 | 18.276 | 1.00 | 0.00 |
| ATOM | 820 | OD1 | ASP | S | 481 | 26.369 | 40.327 | 19.492 | 1.00 | 0.00 |
| ATOM | 821 | OD2 | ASP | S | 481 | 26.942 | 39.279 | 17.706 | 1.00 | 0.00 |
| ATOM | 822 | H | ASP | S | 481 | 27.046 | 40.322 | 15.673 | 1.00 | 0.00 |
| ATOM | 823 | N | GLY | S | 482 | 27.108 | 43.356 | 18.574 | 1.00 | 0.00 |
| ATOM | 824 | CA | GLY | S | 482 | 28.124 | 43.857 | 19.493 | 1.00 | 0.00 |
| ATOM | 825 | C | GLY | S | 482 | 27.657 | 43.799 | 20.930 | 1.00 | 0.00 |
| ATOM | 826 | O | GLY | S | 482 | 27.577 | 44.690 | 21.751 | 1.00 | 0.00 |
| ATOM | 827 | H | GLY | S | 482 | 26.126 | 43.386 | 18.732 | 1.00 | 0.00 |
| ATOM | 828 | N | LYS | S | 483 | 26.891 | 42.738 | 21.202 | 1.00 | 0.00 |
| ATOM | 829 | CA | LYS | S | 483 | 26.034 | 42.850 | 22.376 | 1.00 | 0.00 |
| ATOM | 830 | C | LYS | S | 483 | 26.588 | 42.367 | 23.702 | 1.00 | 0.00 |
| ATOM | 831 | O | LYS | S | 483 | 26.202 | 41.379 | 24.313 | 1.00 | 0.00 |
| ATOM | 832 | CB | LYS | S | 483 | 24.601 | 42.396 | 22.068 | 1.00 | 0.00 |
| ATOM | 833 | CG | LYS | S | 483 | 23.730 | 43.603 | 21.667 | 1.00 | 0.00 |
| ATOM | 834 | CD | LYS | S | 483 | 24.293 | 44.386 | 20.474 | 1.00 | 0.00 |
| ATOM | 835 | CE | LYS | S | 483 | 23.894 | 45.856 | 20.423 | 1.00 | 0.00 |
| ATOM | 836 | NZ | LYS | S | 483 | 24.925 | 46.612 | 19.700 | 1.00 | 0.00 |
| ATOM | 837 | H | LYS | S | 483 | 26.815 | 41.953 | 20.852 | 1.00 | 0.00 |
| ATOM | 838 | 1HZ | LYS | S | 483 | 25.118 | 46.303 | 18.731 | 1.00 | 0.00 |
| ATOM | 839 | 2HZ | LYS | S | 483 | 24.644 | 47.611 | 19.702 | 1.00 | 0.00 |
| ATOM | 840 | 3HZ | LYS | S | 483 | 25.832 | 46.567 | 20.197 | 1.00 | 0.00 |
| ATOM | 841 | N | PHE | S | 484 | 27.520 | 43.235 | 24.159 | 1.00 | 0.00 |
| ATOM | 842 | CA | PHE | S | 484 | 27.960 | 43.319 | 25.554 | 1.00 | 0.00 |
| ATOM | 843 | C | PHE | S | 484 | 28.597 | 42.088 | 26.169 | 1.00 | 0.00 |
| ATOM | 844 | O | PHE | S | 484 | 29.817 | 41.941 | 26.196 | 1.00 | 0.00 |
| ATOM | 845 | CB | PHE | S | 484 | 26.859 | 43.889 | 26.469 | 1.00 | 0.00 |
| ATOM | 846 | CG | PHE | S | 484 | 26.264 | 45.145 | 25.880 | 1.00 | 0.00 |
| ATOM | 847 | CD1 | PHE | S | 484 | 24.969 | 45.092 | 25.320 | 1.00 | 0.00 |
| ATOM | 848 | CD2 | PHE | S | 484 | 27.010 | 46.344 | 25.896 | 1.00 | 0.00 |
| ATOM | 849 | CE1 | PHE | S | 484 | 24.410 | 46.254 | 24.757 | 1.00 | 0.00 |
| ATOM | 850 | CE2 | PHE | S | 484 | 26.452 | 47.507 | 25.334 | 1.00 | 0.00 |
| ATOM | 851 | CZ | PHE | S | 484 | 25.160 | 47.448 | 24.770 | 1.00 | 0.00 |
| ATOM | 852 | H | PHE | S | 484 | 27.823 | 43.941 | 23.520 | 1.00 | 0.00 |
| ATOM | 853 | N | GLY | S | 485 | 27.738 | 41.225 | 26.713 | 1.00 | 0.00 |
| ATOM | 854 | CA | GLY | S | 485 | 28.249 | 40.197 | 27.612 | 1.00 | 0.00 |
| ATOM | 855 | C | GLY | S | 485 | 28.411 | 40.692 | 29.041 | 1.00 | 0.00 |
| ATOM | 856 | O | GLY | S | 485 | 28.290 | 41.876 | 29.354 | 1.00 | 0.00 |
| ATOM | 857 | H | GLY | S | 485 | 26.764 | 41.314 | 26.499 | 1.00 | 0.00 |
| ATOM | 858 | N | THR | S | 486 | 28.696 | 39.718 | 29.908 | 1.00 | 0.00 |
| ATOM | 859 | CA | THR | S | 486 | 28.836 | 39.983 | 31.342 | 1.00 | 0.00 |
| ATOM | 860 | C | THR | S | 486 | 29.868 | 41.035 | 31.736 | 1.00 | 0.00 |
| ATOM | 861 | O | THR | S | 486 | 31.080 | 40.810 | 31.659 | 1.00 | 0.00 |
| ATOM | 862 | CB | THR | S | 486 | 29.138 | 38.663 | 32.043 | 1.00 | 0.00 |
| ATOM | 863 | OG1 | THR | S | 486 | 30.317 | 38.057 | 31.479 | 1.00 | 0.00 |
| ATOM | 864 | CG2 | THR | S | 486 | 27.956 | 37.694 | 31.974 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 865 | H | THR | S | 486 | 28.766 | 38.776 | 29.584 | 1.00 | 0.00 |
| ATOM | 866 | HG1 | THR | S | 486 | 30.834 | 38.812 | 31.197 | 1.00 | 0.00 |
| ATOM | 867 | N | GLN | S | 487 | 29.318 | 42.193 | 32.124 | 1.00 | 0.00 |
| ATOM | 868 | CA | GLN | S | 487 | 30.179 | 43.245 | 32.651 | 1.00 | 0.00 |
| ATOM | 869 | C | GLN | S | 487 | 30.106 | 43.205 | 34.154 | 1.00 | 0.00 |
| ATOM | 870 | O | GLN | S | 487 | 29.129 | 43.643 | 34.759 | 1.00 | 0.00 |
| ATOM | 871 | CB | GLN | S | 487 | 29.749 | 44.632 | 32.175 | 1.00 | 0.00 |
| ATOM | 872 | CG | GLN | S | 487 | 30.811 | 45.687 | 32.505 | 1.00 | 0.00 |
| ATOM | 873 | CD | GLN | S | 487 | 30.210 | 47.073 | 32.441 | 1.00 | 0.00 |
| ATOM | 874 | OE1 | GLN | S | 487 | 29.281 | 47.371 | 31.693 | 1.00 | 0.00 |
| ATOM | 875 | NE2 | GLN | S | 487 | 30.762 | 47.920 | 33.318 | 1.00 | 0.00 |
| ATOM | 876 | H | GLN | S | 487 | 28.338 | 42.224 | 32.287 | 1.00 | 0.00 |
| ATOM | 877 | 1HE2 | GLN | S | 487 | 30.336 | 48.082 | 33.532 | 1.00 | 0.00 |
| ATOM | 878 | 2HE2 | GLN | S | 487 | 31.615 | 47.681 | 33.780 | 1.00 | 0.00 |
| ATOM | 879 | N | GLU | S | 488 | 31.158 | 42.619 | 34.724 | 1.00 | 0.00 |
| ATOM | 880 | CA | GLU | S | 488 | 31.127 | 42.278 | 36.141 | 1.00 | 0.00 |
| ATOM | 881 | C | GLU | S | 488 | 32.221 | 43.028 | 36.887 | 1.00 | 0.00 |
| ATOM | 882 | O | GLU | S | 488 | 32.883 | 43.898 | 36.337 | 1.00 | 0.00 |
| ATOM | 883 | CB | GLU | S | 488 | 31.328 | 40.763 | 36.260 | 1.00 | 0.00 |
| ATOM | 884 | CG | GLU | S | 488 | 30.268 | 39.900 | 35.563 | 1.00 | 0.00 |
| ATOM | 885 | CD | GLU | S | 488 | 30.701 | 38.442 | 35.437 | 1.00 | 0.00 |
| ATOM | 886 | OE1 | GLU | S | 488 | 29.976 | 37.661 | 34.837 | 1.00 | 0.00 |
| ATOM | 887 | OE2 | GLU | S | 488 | 31.769 | 38.059 | 35.899 | 1.00 | 0.00 |
| ATOM | 888 | H | GLU | S | 488 | 31.962 | 42.397 | 34.172 | 1.00 | 0.00 |
| ATOM | 889 | N | ARG | S | 489 | 32.443 | 42.589 | 38.158 | 1.00 | 0.00 |
| ATOM | 890 | CA | ARG | S | 489 | 33.714 | 42.862 | 38.816 | 1.00 | 0.00 |
| ATOM | 891 | C | ARG | S | 489 | 34.960 | 42.573 | 37.977 | 1.00 | 0.00 |
| ATOM | 892 | O | ARG | S | 489 | 34.966 | 41.712 | 37.100 | 1.00 | 0.00 |
| ATOM | 893 | CB | ARG | S | 489 | 33.789 | 42.092 | 40.181 | 1.00 | 0.00 |
| ATOM | 894 | CG | ARG | S | 489 | 34.131 | 40.590 | 40.062 | 1.00 | 0.00 |
| ATOM | 895 | CD | ARG | S | 489 | 33.091 | 39.759 | 39.304 | 1.00 | 0.00 |
| ATOM | 896 | NE | ARG | S | 489 | 33.558 | 38.414 | 38.990 | 1.00 | 0.00 |
| ATOM | 897 | CZ | ARG | S | 489 | 34.127 | 38.127 | 37.796 | 1.00 | 0.00 |
| ATOM | 898 | NH1 | ARG | S | 489 | 34.492 | 36.864 | 37.591 | 1.00 | 0.00 |
| ATOM | 899 | NH2 | ARG | S | 489 | 34.341 | 39.062 | 36.869 | 1.00 | 0.00 |
| ATOM | 900 | H | ARG | S | 489 | 31.582 | 42.134 | 38.588 | 1.00 | 0.00 |
| ATOM | 901 | HE | ARG | S | 489 | 33.434 | 37.732 | 39.710 | 1.00 | 0.00 |
| ATOM | 902 | 1HH1 | ARG | S | 489 | 34.938 | 36.575 | 36.742 | 1.00 | 0.00 |
| ATOM | 903 | 2HH1 | ARG | S | 489 | 34.338 | 36.167 | 38.293 | 1.00 | 0.00 |
| ATOM | 904 | 1HH2 | ARG | S | 489 | 34.770 | 38.917 | 35.972 | 1.00 | 0.00 |
| ATOM | 905 | 2HH2 | ARG | S | 489 | 34.071 | 40.009 | 37.050 | 1.00 | 0.00 |
| ATOM | 906 | N | VAL | S | 490 | 36.020 | 43.314 | 38.309 | 1.00 | 0.00 |
| ATOM | 907 | CA | VAL | S | 490 | 37.302 | 43.139 | 37.620 | 1.00 | 0.00 |
| ATOM | 908 | C | VAL | S | 490 | 38.057 | 41.929 | 38.153 | 1.00 | 0.00 |
| ATOM | 909 | O | VAL | S | 490 | 38.259 | 41.776 | 39.350 | 1.00 | 0.00 |
| ATOM | 910 | CB | VAL | S | 490 | 38.098 | 44.440 | 37.760 | 1.00 | 0.00 |
| ATOM | 911 | CG1 | VAL | S | 490 | 39.477 | 44.400 | 37.095 | 1.00 | 0.00 |
| ATOM | 912 | CG2 | VAL | S | 490 | 37.239 | 45.592 | 37.235 | 1.00 | 0.00 |
| ATOM | 913 | H | VAL | S | 490 | 35.934 | 43.916 | 39.102 | 1.00 | 0.00 |
| ATOM | 914 | N | ASN | S | 491 | 38.388 | 41.029 | 37.222 | 1.00 | 0.00 |
| ATOM | 915 | CA | ASN | S | 491 | 38.824 | 39.684 | 37.593 | 1.00 | 0.00 |
| ATOM | 916 | C | ASN | S | 491 | 39.869 | 39.062 | 36.665 | 1.00 | 0.00 |
| ATOM | 917 | O | ASN | S | 491 | 39.734 | 37.937 | 36.177 | 1.00 | 0.00 |
| ATOM | 918 | CB | ASN | S | 491 | 37.556 | 38.839 | 37.730 | 1.00 | 0.00 |
| ATOM | 919 | CG | ASN | S | 491 | 37.785 | 37.422 | 38.213 | 1.00 | 0.00 |
| ATOM | 920 | OD1 | ASN | S | 491 | 37.196 | 36.480 | 37.692 | 1.00 | 0.00 |
| ATOM | 921 | ND2 | ASN | S | 491 | 38.620 | 37.292 | 39.243 | 1.00 | 0.00 |
| ATOM | 922 | H | ASN | S | 491 | 38.269 | 41.303 | 36.266 | 1.00 | 0.00 |
| ATOM | 923 | 1HD2 | ASN | S | 491 | 39.035 | 38.102 | 39.666 | 1.00 | 0.00 |
| ATOM | 924 | 2HD2 | ASN | S | 491 | 38.836 | 36.393 | 39.616 | 1.00 | 0.00 |
| ATOM | 925 | N | ASN | S | 492 | 40.948 | 39.842 | 36.476 | 1.00 | 0.00 |
| ATOM | 926 | CA | ASN | S | 492 | 42.122 | 39.434 | 35.684 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 927 | C | ASN | S | 492 | 42.688 | 38.054 | 35.993 | 1.00 | 0.00 |
| ATOM | 928 | O | ASN | S | 492 | 43.293 | 37.380 | 35.158 | 1.00 | 0.00 |
| ATOM | 929 | CB | ASN | S | 492 | 43.230 | 40.481 | 35.814 | 1.00 | 0.00 |
| ATOM | 930 | CG | ASN | S | 492 | 44.172 | 40.461 | 34.619 | 1.00 | 0.00 |
| ATOM | 931 | OD1 | ASN | S | 492 | 44.716 | 39.438 | 34.198 | 1.00 | 0.00 |
| ATOM | 932 | ND2 | ASN | S | 492 | 44.431 | 41.683 | 34.142 | 1.00 | 0.00 |
| ATOM | 933 | H | ASN | S | 492 | 40.893 | 40.771 | 36.840 | 1.00 | 0.00 |
| ATOM | 934 | 1HD2 | ASN | S | 492 | 43.794 | 42.429 | 34.351 | 1.00 | 0.00 |
| ATOM | 935 | 2HD2 | ASN | S | 492 | 45.239 | 41.824 | 33.568 | 1.00 | 0.00 |
| ATOM | 936 | N | SER | S | 493 | 42.415 | 37.633 | 37.233 | 1.00 | 0.00 |
| ATOM | 937 | CA | SER | S | 493 | 42.701 | 36.284 | 37.719 | 1.00 | 0.00 |
| ATOM | 938 | C | SER | S | 493 | 42.368 | 35.129 | 36.775 | 1.00 | 0.00 |
| ATOM | 939 | O | SER | S | 493 | 43.136 | 34.183 | 36.634 | 1.00 | 0.00 |
| ATOM | 940 | CB | SER | S | 493 | 42.011 | 36.142 | 39.072 | 1.00 | 0.00 |
| ATOM | 941 | OG | SER | S | 493 | 41.927 | 37.443 | 39.682 | 1.00 | 0.00 |
| ATOM | 942 | H | SER | S | 493 | 42.022 | 38.303 | 37.867 | 1.00 | 0.00 |
| ATOM | 943 | HG | SER | S | 493 | 42.286 | 37.350 | 40.559 | 1.00 | 0.00 |
| ATOM | 944 | N | ASN | S | 494 | 41.213 | 35.281 | 36.104 | 1.00 | 0.00 |
| ATOM | 945 | CA | ASN | S | 494 | 41.027 | 34.543 | 34.853 | 1.00 | 0.00 |
| ATOM | 946 | C | ASN | S | 494 | 40.323 | 35.387 | 33.818 | 1.00 | 0.00 |
| ATOM | 947 | O | ASN | S | 494 | 39.302 | 35.028 | 33.238 | 1.00 | 0.00 |
| ATOM | 948 | CB | ASN | S | 494 | 40.329 | 33.183 | 34.935 | 1.00 | 0.00 |
| ATOM | 949 | CG | ASN | S | 494 | 40.528 | 32.424 | 33.674 | 1.00 | 0.00 |
| ATOM | 950 | OD1 | ASN | S | 494 | 41.642 | 32.254 | 33.189 | 1.00 | 0.00 |
| ATOM | 951 | ND2 | ASN | S | 494 | 39.406 | 31.969 | 33.111 | 1.00 | 0.00 |
| ATOM | 952 | H | ASN | S | 494 | 40.574 | 36.001 | 36.373 | 1.00 | 0.00 |
| ATOM | 953 | 1HD2 | ASN | S | 494 | 38.508 | 32.176 | 33.491 | 1.00 | 0.00 |
| ATOM | 954 | 2HD2 | ASN | S | 494 | 49.496 | 31.404 | 32.295 | 1.00 | 0.00 |
| ATOM | 955 | N | LYS | S | 495 | 40.936 | 36.566 | 33.628 | 1.00 | 0.00 |
| ATOM | 956 | CA | LYS | S | 495 | 40.699 | 37.386 | 32.439 | 1.00 | 0.00 |
| ATOM | 957 | C | LYS | S | 495 | 39.244 | 37.796 | 32.221 | 1.00 | 0.00 |
| ATOM | 958 | O | LYS | S | 495 | 38.790 | 38.143 | 31.135 | 1.00 | 0.00 |
| ATOM | 959 | CB | LYS | S | 495 | 41.345 | 36.706 | 31.215 | 1.00 | 0.00 |
| ATOM | 960 | CG | LYS | S | 495 | 42.886 | 36.613 | 31.262 | 1.00 | 0.00 |
| ATOM | 961 | CD | LYS | S | 495 | 43.548 | 35.637 | 32.256 | 1.00 | 0.00 |
| ATOM | 962 | CE | LYS | S | 495 | 45.044 | 35.862 | 32.553 | 1.00 | 0.00 |
| ATOM | 963 | NZ | LYS | S | 495 | 45.285 | 37.043 | 33.400 | 1.00 | 0.00 |
| ATOM | 964 | H | LYS | S | 495 | 41.734 | 36.708 | 34.209 | 1.00 | 0.00 |
| ATOM | 965 | 1HZ | LYS | S | 495 | 46.281 | 37.042 | 33.677 | 1.00 | 0.00 |
| ATOM | 966 | 2HZ | LYS | S | 495 | 45.091 | 37.966 | 32.947 | 1.00 | 0.00 |
| ATOM | 967 | 3HZ | LYS | S | 495 | 44.704 | 36.986 | 34.262 | 1.00 | 0.00 |
| ATOM | 968 | N | LYS | S | 496 | 38.536 | 37.753 | 33.358 | 1.00 | 0.00 |
| ATOM | 969 | CA | LYS | S | 496 | 37.087 | 37.893 | 33.353 | 1.00 | 0.00 |
| ATOM | 970 | C | LYS | S | 496 | 36.677 | 39.307 | 33.697 | 1.00 | 0.00 |
| ATOM | 971 | O | LYS | S | 496 | 35.930 | 39.558 | 34.645 | 1.00 | 0.00 |
| ATOM | 972 | CB | LYS | S | 496 | 36.489 | 36.881 | 34.336 | 1.00 | 0.00 |
| ATOM | 973 | CG | LYS | S | 496 | 35.307 | 36.028 | 33.852 | 1.00 | 0.00 |
| ATOM | 974 | CD | LYS | S | 496 | 33.996 | 36.775 | 33.581 | 1.00 | 0.00 |
| ATOM | 975 | CE | LYS | S | 496 | 32.821 | 35.799 | 33.426 | 1.00 | 0.00 |
| ATOM | 976 | NZ | LYS | S | 496 | 31.583 | 36.529 | 33.159 | 1.00 | 0.00 |
| ATOM | 977 | H | LYS | S | 496 | 39.027 | 37.684 | 34.226 | 1.00 | 0.00 |
| ATOM | 978 | 1HZ | LYS | S | 496 | 31.495 | 36.874 | 32.176 | 1.00 | 0.00 |
| ATOM | 979 | 2HZ | LYS | S | 496 | 30.770 | 35.928 | 33.359 | 1.00 | 0.00 |
| ATOM | 980 | 3HZ | LYS | S | 496 | 31.472 | 37.312 | 33.841 | 1.00 | 0.00 |
| ATOM | 981 | N | GLU | S | 497 | 37.207 | 40.211 | 32.865 | 1.00 | 0.00 |
| ATOM | 982 | CA | GLU | S | 497 | 36.952 | 41.634 | 33.103 | 1.00 | 0.00 |
| ATOM | 983 | C | GLU | S | 497 | 35.622 | 42.124 | 32.533 | 1.00 | 0.00 |
| ATOM | 984 | O | GLU | S | 497 | 35.004 | 43.074 | 33.020 | 1.00 | 0.00 |
| ATOM | 985 | CB | GLU | S | 497 | 38.105 | 42.477 | 32.547 | 1.00 | 0.00 |
| ATOM | 986 | CG | GLU | S | 497 | 39.519 | 41.866 | 32.584 | 1.00 | 0.00 |
| ATOM | 987 | CD | GLU | S | 497 | 40.227 | 42.044 | 33.917 | 1.00 | 0.00 |
| ATOM | 988 | OE1 | GLU | S | 497 | 39.593 | 41.946 | 34.959 | 1.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 989 | OE2 | GLU | S | 497 | 41.432 | 42.278 | 33.917 | 1.00 | 0.00 |
| ATOM | 990 | H | GLU | S | 497 | 37.776 | 39.884 | 32.109 | 1.00 | 0.00 |
| ATOM | 991 | N | TRP | S | 498 | 35.240 | 41.398 | 31.465 | 1.00 | 0.00 |
| ATOM | 992 | CA | TRP | S | 498 | 33.956 | 41.498 | 30.777 | 1.00 | 0.00 |
| ATOM | 993 | C | TRP | S | 498 | 33.936 | 40.243 | 29.905 | 1.00 | 0.00 |
| ATOM | 994 | O | TRP | S | 498 | 35.003 | 39.779 | 29.509 | 1.00 | 0.00 |
| ATOM | 995 | CB | TRP | S | 498 | 34.004 | 42.780 | 29.925 | 1.00 | 0.00 |
| ATOM | 996 | CG | TRP | S | 498 | 32.685 | 43.096 | 29.499 | 1.00 | 0.00 |
| ATOM | 997 | CD1 | TRP | S | 498 | 31.440 | 42.782 | 29.300 | 1.00 | 0.00 |
| ATOM | 998 | CD2 | TRP | S | 498 | 32.458 | 44.788 | 29.182 | 1.00 | 0.00 |
| ATOM | 999 | NE1 | TRP | S | 498 | 30.492 | 43.674 | 28.900 | 1.00 | 0.00 |
| ATOM | 1000 | CE2 | TRP | S | 498 | 31.076 | 44.929 | 28.815 | 1.00 | 0.00 |
| ATOM | 1001 | CE3 | TRP | S | 498 | 33.305 | 45.916 | 29.164 | 1.00 | 0.00 |
| ATOM | 1002 | CZ2 | TRP | S | 498 | 30.568 | 46.194 | 28.448 | 1.00 | 0.00 |
| ATOM | 1003 | CZ3 | TRP | S | 498 | 32.785 | 47.172 | 28.787 | 1.00 | 0.00 |
| ATOM | 1004 | CH2 | TRP | S | 498 | 31.425 | 47.313 | 28.435 | 1.00 | 0.00 |
| ATOM | 1005 | H | TRP | S | 498 | 35.880 | 40.725 | 31.096 | 1.00 | 0.00 |
| ATOM | 1006 | HE1 | TRP | S | 498 | 29.557 | 43.437 | 28.700 | 1.00 | 0.00 |
| ATOM | 1007 | N | ASN | S | 499 | 32.758 | 39.714 | 29.566 | 1.00 | 0.00 |
| ATOM | 1008 | CA | ASN | S | 499 | 32.805 | 38.369 | 28.362 | 1.00 | 0.00 |
| ATOM | 1009 | C | ASN | S | 499 | 32.691 | 39.767 | 27.138 | 1.00 | 0.00 |
| ATOM | 1010 | O | ASN | S | 499 | 32.796 | 40.981 | 27.306 | 1.00 | 0.00 |
| ATOM | 1011 | CB | ASN | S | 499 | 31.752 | 37.757 | 28.408 | 1.00 | 0.00 |
| ATOM | 1012 | CG | ASN | S | 499 | 32.305 | 36.575 | 29.190 | 1.00 | 0.00 |
| ATOM | 1013 | OD1 | ASN | S | 499 | 32.180 | 36.466 | 30.413 | 1.00 | 0.00 |
| ATOM | 1014 | ND2 | ASN | S | 499 | 32.950 | 35.681 | 28.431 | 1.00 | 0.00 |
| ATOM | 1015 | H | ASN | S | 499 | 31.940 | 40.118 | 29.906 | 1.00 | 0.00 |
| ATOM | 1016 | 1HD2 | ASN | S | 499 | 33.356 | 34.846 | 28.794 | 1.00 | 0.00 |
| ATOM | 1017 | 2HD2 | ASN | S | 499 | 33.006 | 35.809 | 27.434 | 1.00 | 0.00 |
| ATOM | 1018 | N | GLY | S | 500 | 32.490 | 39.180 | 25.943 | 1.00 | 0.00 |
| ATOM | 1019 | CA | GLY | S | 500 | 31.984 | 39.907 | 24.767 | 1.00 | 0.00 |
| ATOM | 1020 | C | GLY | S | 500 | 32.716 | 41.156 | 24.297 | 1.00 | 0.00 |
| ATOM | 1021 | O | GLY | S | 500 | 33.520 | 41.169 | 23.361 | 1.00 | 0.00 |
| ATOM | 1022 | H | GLY | S | 500 | 32.683 | 38.198 | 25.848 | 1.00 | 0.00 |
| ATOM | 1023 | N | MET | S | 501 | 32.364 | 42.247 | 24.990 | 1.00 | 0.00 |
| ATOM | 1024 | CA | MET | S | 501 | 32.956 | 43.558 | 24.736 | 1.00 | 0.00 |
| ATOM | 1025 | C | MET | S | 501 | 34.433 | 43.655 | 25.046 | 1.00 | 0.00 |
| ATOM | 1026 | O | MET | S | 501 | 35.164 | 44.443 | 24.457 | 1.00 | 0.00 |
| ATOM | 1027 | CB | MET | S | 501 | 32.216 | 44.625 | 25.534 | 1.00 | 0.00 |
| ATOM | 1028 | CG | MET | S | 501 | 31.048 | 45.302 | 24.820 | 1.00 | 0.00 |
| ATOM | 1029 | SD | MET | S | 501 | 31.600 | 46.529 | 23.626 | 1.00 | 0.00 |
| ATOM | 1030 | CE | MET | S | 501 | 29.975 | 47.174 | 23.209 | 1.00 | 0.00 |
| ATOM | 1031 | H | MET | S | 501 | 31.791 | 42.053 | 25.789 | 1.00 | 0.00 |
| ATOM | 1032 | N | MET | S | 502 | 34.851 | 42.835 | 26.014 | 1.00 | 0.00 |
| ATOM | 1033 | CA | MET | S | 502 | 36.282 | 42.712 | 26.284 | 1.00 | 0.00 |
| ATOM | 1034 | C | MET | S | 502 | 36.746 | 41.273 | 26.211 | 1.00 | 0.00 |
| ATOM | 1035 | O | MET | S | 502 | 37.864 | 40.947 | 25.812 | 1.00 | 0.00 |
| ATOM | 1036 | CB | MET | S | 502 | 36.643 | 43.306 | 27.642 | 1.00 | 0.00 |
| ATOM | 1037 | CG | MET | S | 502 | 38.147 | 43.352 | 27.920 | 1.00 | 0.00 |
| ATOM | 1038 | SD | MET | S | 502 | 38.532 | 43.813 | 29.614 | 1.00 | 0.00 |
| ATOM | 1039 | CE | MET | S | 502 | 37.385 | 45.187 | 29.807 | 1.00 | 0.00 |
| ATOM | 1040 | H | MET | S | 502 | 34.174 | 42.197 | 26.376 | 1.00 | 0.00 |
| ATOM | 1041 | N | GLY | S | 503 | 35.817 | 40.387 | 26.596 | 1.00 | 0.00 |
| ATOM | 1042 | CA | GLY | S | 503 | 36.003 | 38.961 | 26.320 | 1.00 | 0.00 |
| ATOM | 1043 | C | GLY | S | 503 | 36.434 | 38.700 | 24.892 | 1.00 | 0.00 |
| ATOM | 1044 | O | GLY | S | 503 | 37.442 | 38.056 | 24.625 | 1.00 | 0.00 |
| ATOM | 1045 | H | GLY | S | 503 | 34.996 | 40.752 | 27.033 | 1.00 | 0.00 |
| ATOM | 1046 | N | GLU | S | 504 | 35.691 | 39.328 | 23.970 | 1.00 | 0.00 |
| ATOM | 1047 | CA | GLU | S | 504 | 36.150 | 39.086 | 22.609 | 1.00 | 0.00 |
| ATOM | 1048 | C | GLU | S | 504 | 37.179 | 40.073 | 22.093 | 1.00 | 0.00 |
| ATOM | 1049 | O | GLU | S | 504 | 37.780 | 39.895 | 21.033 | 1.00 | 0.00 |
| ATOM | 1050 | CB | GLU | S | 504 | 34.988 | 38.831 | 21.642 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1051 CG | GLU | S | 504 | 33.834 | 37.921 | 22.123 | 1.00 | 0.00 |
| ATOM | 1052 CD | GLU | S | 504 | 34.226 | 36.936 | 23.221 | 1.00 | 0.00 |
| ATOM | 1053 OE1 | GLU | S | 504 | 35.132 | 36.125 | 23.027 | 1.00 | 0.00 |
| ATOM | 1054 OE2 | GLU | S | 504 | 33.633 | 37.013 | 24.295 | 1.00 | 0.00 |
| ATOM | 1055 H | GLU | S | 504 | 34.930 | 39.930 | 24.218 | 1.00 | 0.00 |
| ATOM | 1056 N | LEU | S | 505 | 37.411 | 41.099 | 22.928 | 1.00 | 0.00 |
| ATOM | 1057 CA | LEU | S | 505 | 38.707 | 41.754 | 22.779 | 1.00 | 0.00 |
| ATOM | 1058 C | LEU | S | 505 | 39.898 | 40.881 | 23.152 | 1.00 | 0.00 |
| ATOM | 1059 O | LEU | S | 505 | 41.013 | 41.113 | 22.684 | 1.00 | 0.00 |
| ATOM | 1060 CB | LEU | S | 505 | 38.782 | 43.071 | 23.558 | 1.00 | 0.00 |
| ATOM | 1061 CG | LEU | S | 505 | 38.622 | 44.332 | 22.707 | 1.00 | 0.00 |
| ATOM | 1062 CD1 | LEU | S | 505 | 37.240 | 44.459 | 22.075 | 1.00 | 0.00 |
| ATOM | 1063 CD2 | LEU | S | 505 | 38.980 | 45.587 | 23.497 | 1.00 | 0.00 |
| ATOM | 1064 H | LEU | S | 505 | 36.889 | 41.220 | 23.766 | 1.00 | 0.00 |
| ATOM | 1065 N | LEU | S | 506 | 39.629 | 39.894 | 24.022 | 1.00 | 0.00 |
| ATOM | 1066 CA | LEU | S | 506 | 40.672 | 38.933 | 24.388 | 1.00 | 0.00 |
| ATOM | 1067 C | LEU | S | 506 | 40.618 | 37.641 | 23.584 | 1.00 | 0.00 |
| ATOM | 1068 O | LEU | S | 506 | 41.566 | 36.862 | 23.520 | 1.00 | 0.00 |
| ATOM | 1069 CB | LEU | S | 506 | 40.618 | 38.639 | 25.890 | 1.00 | 0.00 |
| ATOM | 1070 CG | LEU | S | 506 | 40.759 | 39.887 | 26.771 | 1.00 | 0.00 |
| ATOM | 1071 CD1 | LEU | S | 506 | 40.437 | 39.587 | 28.235 | 1.00 | 0.00 |
| ATOM | 1072 CD2 | LEU | S | 506 | 42.117 | 40.574 | 26.606 | 1.00 | 0.00 |
| ATOM | 1073 H | LEU | S | 506 | 38.673 | 39.736 | 24.260 | 1.00 | 0.00 |
| ATOM | 1074 N | SER | S | 507 | 39.466 | 37.438 | 22.920 | 1.00 | 0.00 |
| ATOM | 1075 CA | SER | S | 507 | 39.417 | 36.267 | 22.046 | 1.00 | 0.00 |
| ATOM | 1076 C | SER | S | 507 | 39.655 | 36.574 | 20.575 | 1.00 | 0.00 |
| ATOM | 1077 O | SER | S | 507 | 39.881 | 35.963 | 19.755 | 1.00 | 0.00 |
| ATOM | 1078 CB | SER | S | 507 | 38.136 | 35.443 | 22.246 | 1.00 | 0.00 |
| ATOM | 1079 OG | SER | S | 507 | 37.864 | 35.223 | 23.644 | 1.00 | 0.00 |
| ATOM | 1080 H | SER | S | 507 | 38.677 | 38.015 | 23.122 | 1.00 | 0.00 |
| ATOM | 1081 HG | SER | S | 507 | 37.087 | 35.763 | 23.831 | 1.00 | 0.00 |
| ATOM | 1082 N | GLY | S | 508 | 39.638 | 37.874 | 20.242 | 1.00 | 0.00 |
| ATOM | 1083 CA | GLY | S | 508 | 40.126 | 38.161 | 18.897 | 1.00 | 0.00 |
| ATOM | 1084 C | GLY | S | 508 | 39.047 | 38.459 | 17.877 | 1.00 | 0.00 |
| ATOM | 1085 O | GLY | S | 508 | 39.306 | 39.092 | 16.857 | 1.00 | 0.00 |
| ATOM | 1086 H | GLY | S | 508 | 39.259 | 38.585 | 20.832 | 1.00 | 0.00 |
| ATOM | 1087 N | GLN | S | 509 | 37.817 | 38.029 | 18.211 | 1.00 | 0.00 |
| ATOM | 1088 CA | GLN | S | 509 | 36.652 | 38.500 | 17.459 | 1.00 | 0.00 |
| ATOM | 1089 C | GLN | S | 509 | 36.620 | 40.014 | 17.272 | 1.00 | 0.00 |
| ATOM | 1090 O | GLN | S | 509 | 36.167 | 40.532 | 16.251 | 1.00 | 0.00 |
| ATOM | 1091 CB | GLN | S | 509 | 35.350 | 38.078 | 18.152 | 1.00 | 0.00 |
| ATOM | 1092 CG | GLN | S | 509 | 34.857 | 36.629 | 18.019 | 1.00 | 0.00 |
| ATOM | 1093 CD | GLN | S | 509 | 35.827 | 35.614 | 18.594 | 1.00 | 0.00 |
| ATOM | 1094 OE1 | GLN | S | 509 | 36.628 | 35.034 | 17.870 | 1.00 | 0.00 |
| ATOM | 1095 NE2 | GLN | S | 509 | 35.690 | 35.369 | 19.905 | 1.00 | 0.00 |
| ATOM | 1096 H | GLN | S | 509 | 37.723 | 37.391 | 18.972 | 1.00 | 0.00 |
| ATOM | 1097 1HE2 | GLN | S | 509 | 36.196 | 34.595 | 20.296 | 1.00 | 0.00 |
| ATOM | 1098 2HE2 | GLN | S | 509 | 35.067 | 35.891 | 20.499 | 1.00 | 0.00 |
| ATOM | 1099 N | ALA | S | 510 | 37.103 | 40.688 | 18.327 | 1.00 | 0.00 |
| ATOM | 1100 CA | ALA | S | 510 | 37.127 | 42.141 | 18.383 | 1.00 | 0.00 |
| ATOM | 1101 C | ALA | S | 510 | 38.423 | 42.687 | 18.956 | 1.00 | 0.00 |
| ATOM | 1102 O | ALA | S | 510 | 39.100 | 42.089 | 19.800 | 1.00 | 0.00 |
| ATOM | 1103 CB | ALA | S | 510 | 35.950 | 42.648 | 19.217 | 1.00 | 0.00 |
| ATOM | 1104 H | ALA | S | 510 | 37.513 | 40.172 | 19.080 | 1.00 | 0.00 |
| ATOM | 1105 N | ASP | S | 511 | 38.741 | 43.871 | 18.438 | 1.00 | 0.00 |
| ATOM | 1106 CA | ASP | S | 511 | 39.993 | 44.506 | 18.835 | 1.00 | 0.00 |
| ATOM | 1107 C | ASP | S | 511 | 39.741 | 45.753 | 19.657 | 1.00 | 0.00 |
| ATOM | 1108 O | ASP | S | 511 | 40.434 | 46.132 | 20.604 | 1.00 | 0.00 |
| ATOM | 1109 CB | ASP | S | 511 | 40.796 | 44.925 | 17.602 | 1.00 | 0.00 |
| ATOM | 1110 CG | ASP | S | 511 | 40.974 | 43.821 | 16.580 | 1.00 | 0.00 |
| ATOM | 1111 OD1 | ASP | S | 511 | 42.005 | 43.165 | 16.575 | 1.00 | 0.00 |
| ATOM | 1112 OD2 | ASP | S | 511 | 40.093 | 43.623 | 15.757 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1113 H | ASP | S | 511 | 38.130 | 44.283 | 17.765 | 1.00 | 0.00 |
| ATOM | 1114 N | MET | S | 512 | 38.698 | 46.433 | 19.191 | 1.00 | 0.00 |
| ATOM | 1115 CA | MET | S | 512 | 38.498 | 47.774 | 19.688 | 1.00 | 0.00 |
| ATOM | 1116 C | MET | S | 512 | 37.080 | 48.092 | 20.059 | 1.00 | 0.00 |
| ATOM | 1117 O | MET | S | 512 | 36.129 | 48.128 | 19.268 | 1.00 | 0.00 |
| ATOM | 1118 CB | MET | S | 512 | 39.022 | 48.805 | 18.693 | 1.00 | 0.00 |
| ATOM | 1119 CG | MET | S | 512 | 38.666 | 48.536 | 17.234 | 1.00 | 0.00 |
| ATOM | 1120 SD | MET | S | 512 | 38.992 | 49.967 | 16.203 | 1.00 | 0.00 |
| ATOM | 1121 CE | MET | S | 512 | 40.631 | 50.353 | 16.809 | 1.00 | 0.00 |
| ATOM | 1122 H | MET | S | 512 | 38.125 | 46.075 | 18.459 | 1.00 | 0.00 |
| ATOM | 1123 N | ILE | S | 513 | 36.941 | 48.420 | 21.349 | 1.00 | 0.00 |
| ATOM | 1124 CA | ILE | S | 513 | 35.709 | 49.155 | 21.593 | 1.00 | 0.00 |
| ATOM | 1125 C | ILE | S | 513 | 35.877 | 50.555 | 21.027 | 1.00 | 0.00 |
| ATOM | 1126 O | ILE | S | 513 | 36.906 | 51.194 | 21.227 | 1.00 | 0.00 |
| ATOM | 1127 CB | ILE | S | 513 | 35.287 | 49.151 | 23.065 | 1.00 | 0.00 |
| ATOM | 1128 CG1 | ILE | S | 513 | 35.569 | 47.784 | 23.703 | 1.00 | 0.00 |
| ATOM | 1129 CG2 | ILE | S | 513 | 33.794 | 49.489 | 23.123 | 1.00 | 0.00 |
| ATOM | 1130 CD1 | ILE | S | 513 | 35.265 | 47.710 | 25.201 | 1.00 | 0.00 |
| ATOM | 1131 H | ILE | S | 513 | 37.770 | 48.460 | 21.915 | 1.00 | 0.00 |
| ATOM | 1132 N | VAL | S | 514 | 34.860 | 50.884 | 20.199 | 1.00 | 0.00 |
| ATOM | 1133 CA | VAL | S | 514 | 34.806 | 52.218 | 19.590 | 1.00 | 0.00 |
| ATOM | 1134 C | VAL | S | 514 | 33.434 | 52.836 | 19.742 | 1.00 | 0.00 |
| ATOM | 1135 O | VAL | S | 514 | 33.302 | 54.054 | 19.792 | 1.00 | 0.00 |
| ATOM | 1136 CB | VAL | S | 514 | 35.221 | 52.237 | 18.114 | 1.00 | 0.00 |
| ATOM | 1137 CG1 | VAL | S | 514 | 35.323 | 53.658 | 17.552 | 1.00 | 0.00 |
| ATOM | 1138 CG2 | VAL | S | 514 | 36.517 | 51.478 | 17.891 | 1.00 | 0.00 |
| ATOM | 1139 H | VAL | S | 514 | 34.155 | 50.182 | 20.070 | 1.00 | 0.00 |
| ATOM | 1140 N | ALA | S | 515 | 32.431 | 51.930 | 19.924 | 1.00 | 0.00 |
| ATOM | 1141 CA | ALA | S | 515 | 31.175 | 52.379 | 20.535 | 1.00 | 0.00 |
| ATOM | 1142 C | ALA | S | 515 | 31.484 | 53.244 | 21.729 | 1.00 | 0.00 |
| ATOM | 1143 O | ALA | S | 515 | 32.246 | 52.778 | 22.579 | 1.00 | 0.00 |
| ATOM | 1144 CB | ALA | S | 515 | 30.421 | 51.184 | 21.094 | 1.00 | 0.00 |
| ATOM | 1145 H | ALA | S | 515 | 32.516 | 50.969 | 19.660 | 1.00 | 0.00 |
| ATOM | 1146 N | PRO | S | 516 | 30.967 | 54.505 | 21.705 | 1.00 | 0.00 |
| ATOM | 1147 CA | PRO | S | 516 | 31.407 | 55.539 | 22.650 | 1.00 | 0.00 |
| ATOM | 1148 C | PRO | S | 516 | 31.682 | 55.021 | 24.041 | 1.00 | 0.00 |
| ATOM | 1149 O | PRO | S | 516 | 30.795 | 54.749 | 24.854 | 1.00 | 0.00 |
| ATOM | 1150 CB | PRO | S | 516 | 30.288 | 56.574 | 22.536 | 1.00 | 0.00 |
| ATOM | 1151 CG | PRO | S | 516 | 29.910 | 56.506 | 21.057 | 1.00 | 0.00 |
| ATOM | 1152 CD | PRO | S | 516 | 29.985 | 55.013 | 20.748 | 1.00 | 0.00 |
| ATOM | 1153 N | LEU | S | 517 | 32.982 | 54.798 | 24.236 | 1.00 | 0.00 |
| ATOM | 1154 CA | LEU | S | 517 | 33.429 | 53.996 | 25.364 | 1.00 | 0.00 |
| ATOM | 1155 C | LEU | S | 517 | 33.909 | 54.921 | 26.432 | 1.00 | 0.00 |
| ATOM | 1156 O | LEU | S | 517 | 34.367 | 56.031 | 26.176 | 1.00 | 0.00 |
| ATOM | 1157 CB | LEU | S | 517 | 34.550 | 53.045 | 24.938 | 1.00 | 0.00 |
| ATOM | 1158 CG | LEU | S | 517 | 34.978 | 52.093 | 26.058 | 1.00 | 0.00 |
| ATOM | 1159 CD1 | LEU | S | 517 | 33.905 | 51.060 | 26.395 | 1.00 | 0.00 |
| ATOM | 1160 CD2 | LEU | S | 517 | 36.344 | 51.483 | 25.801 | 1.00 | 0.00 |
| ATOM | 1161 H | LEU | S | 517 | 33.647 | 55.225 | 23.619 | 1.00 | 0.00 |
| ATOM | 1162 N | THR | S | 518 | 33.738 | 54.470 | 27.667 | 1.00 | 0.00 |
| ATOM | 1163 CA | THR | S | 518 | 34.288 | 55.278 | 28.749 | 1.00 | 0.00 |
| ATOM | 1164 C | THR | S | 518 | 35.678 | 54.736 | 29.036 | 1.00 | 0.00 |
| ATOM | 1165 O | THR | S | 518 | 35.893 | 53.543 | 28.802 | 1.00 | 0.00 |
| ATOM | 1166 CB | THR | S | 518 | 33.327 | 55.136 | 29.926 | 1.00 | 0.00 |
| ATOM | 1167 OG1 | THR | S | 518 | 32.044 | 54.658 | 29.457 | 1.00 | 0.00 |
| ATOM | 1168 CG2 | THR | S | 518 | 33.102 | 56.482 | 30.607 | 1.00 | 0.00 |
| ATOM | 1169 H | THR | S | 518 | 33.465 | 53.513 | 27.815 | 1.00 | 0.00 |
| ATOM | 1170 HG1 | THR | S | 518 | 32.146 | 53.713 | 29.268 | 1.00 | 0.00 |
| ATOM | 1171 N | ILE | S | 519 | 36.629 | 55.579 | 29.477 | 1.00 | 0.00 |
| ATOM | 1172 CA | ILE | S | 519 | 37.876 | 54.878 | 29.799 | 1.00 | 0.00 |
| ATOM | 1173 C | ILE | S | 519 | 37.926 | 54.432 | 31.242 | 1.00 | 0.00 |
| ATOM | 1174 O | ILE | S | 519 | 38.350 | 55.170 | 32.133 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1175 CB | ILE | S | 519 | 39.148 | 55.657 | 29.433 | 1.00 | 0.00 |
| ATOM | 1176 CG1 | ILE | S | 519 | 39.143 | 56.077 | 27.967 | 1.00 | 0.00 |
| ATOM | 1177 CG2 | ILE | S | 519 | 40.404 | 54.813 | 29.708 | 1.00 | 0.00 |
| ATOM | 1178 CD1 | ILE | S | 519 | 40.346 | 56.975 | 27.687 | 1.00 | 0.00 |
| ATOM | 1179 H | ILE | S | 519 | 36.471 | 56.570 | 29.541 | 1.00 | 0.00 |
| ATOM | 1180 N | ASN | S | 520 | 37.463 | 53.190 | 31.410 | 1.00 | 0.00 |
| ATOM | 1181 CA | ASN | S | 520 | 37.777 | 52.505 | 32.657 | 1.00 | 0.00 |
| ATOM | 1182 C | ASN | S | 520 | 39.258 | 52.338 | 32.792 | 1.00 | 0.00 |
| ATOM | 1183 O | ASN | S | 520 | 39.928 | 51.986 | 31.819 | 1.00 | 0.00 |
| ATOM | 1184 CB | ASN | S | 520 | 37.170 | 51.118 | 32.690 | 1.00 | 0.00 |
| ATOM | 1185 CG | ASN | S | 520 | 35.811 | 51.199 | 33.303 | 1.00 | 0.00 |
| ATOM | 1186 OD1 | ASN | S | 520 | 34.765 | 51.198 | 32.661 | 1.00 | 0.00 |
| ATOM | 1187 ND2 | ASN | S | 520 | 35.844 | 51.266 | 34.624 | 1.00 | 0.00 |
| ATOM | 1188 H | ASN | S | 520 | 37.109 | 52.720 | 30.603 | 1.00 | 0.00 |
| ATOM | 1189 1HD2 | ASN | S | 520 | 34.970 | 51.383 | 35.093 | 1.00 | 0.00 |
| ATOM | 1190 2HD2 | ASN | S | 520 | 36.680 | 51.229 | 35.171 | 1.00 | 0.00 |
| ATOM | 1191 N | ASN | S | 521 | 39.723 | 52.578 | 34.025 | 1.00 | 0.00 |
| ATOM | 1192 CA | ASN | S | 521 | 41.154 | 52.386 | 34.264 | 1.00 | 0.00 |
| ATOM | 1193 C | ASN | S | 521 | 41.570 | 50.954 | 34.142 | 1.00 | 0.00 |
| ATOM | 1194 O | ASN | S | 521 | 42.686 | 50.634 | 33.756 | 1.00 | 0.00 |
| ATOM | 1195 CB | ASN | S | 521 | 41.621 | 52.830 | 35.645 | 1.00 | 0.00 |
| ATOM | 1196 CG | ASN | S | 521 | 41.265 | 54.263 | 35.925 | 1.00 | 0.00 |
| ATOM | 1197 OD1 | ASN | S | 521 | 40.844 | 54.594 | 37.027 | 1.00 | 0.00 |
| ATOM | 1198 ND2 | ASN | S | 521 | 41.424 | 55.107 | 34.893 | 1.00 | 0.00 |
| ATOM | 1199 H | ASN | S | 521 | 39.069 | 52.659 | 34.773 | 1.00 | 0.00 |
| ATOM | 1200 1HD2 | ASN | S | 521 | 41.150 | 56.063 | 35.029 | 1.00 | 0.00 |
| ATOM | 1201 2HD2 | ASN | S | 521 | 41.747 | 54.756 | 34.011 | 1.00 | 0.00 |
| ATOM | 1202 N | GLU | S | 522 | 40.602 | 50.104 | 34.481 | 1.00 | 0.00 |
| ATOM | 1203 CA | GLU | S | 522 | 40.763 | 58.653 | 34.431 | 1.00 | 0.00 |
| ATOM | 1204 C | GLU | S | 522 | 40.928 | 48.141 | 33.014 | 1.00 | 0.00 |
| ATOM | 1205 O | GLU | S | 522 | 41.694 | 47.218 | 32.720 | 1.00 | 0.00 |
| ATOM | 1206 CB | GLU | S | 522 | 39.592 | 47.980 | 35.150 | 1.00 | 0.00 |
| ATOM | 1207 CG | GLU | S | 522 | 39.434 | 48.372 | 36.632 | 1.00 | 0.00 |
| ATOM | 1208 CD | GLU | S | 522 | 39.027 | 49.826 | 36.806 | 1.00 | 0.00 |
| ATOM | 1209 OE1 | GLU | S | 522 | 28.142 | 50.302 | 36.099 | 1.00 | 0.00 |
| ATOM | 1210 OE2 | GLU | S | 522 | 39.629 | 50.517 | 37.619 | 1.00 | 0.00 |
| ATOM | 1211 H | GLU | S | 522 | 39.738 | 50.500 | 34.785 | 1.00 | 0.00 |
| ATOM | 1212 N | ARG | S | 523 | 40.230 | 48.882 | 32.126 | 1.00 | 0.00 |
| ATOM | 1213 CA | ARG | S | 523 | 40.579 | 48.782 | 30.716 | 1.00 | 0.00 |
| ATOM | 1214 C | ARG | S | 523 | 41.978 | 49.290 | 30.457 | 1.00 | 0.00 |
| ATOM | 1215 O | ARG | S | 523 | 42.842 | 48.510 | 30.084 | 1.00 | 0.00 |
| ATOM | 1216 CB | ARG | S | 523 | 39.532 | 49.457 | 29.830 | 1.00 | 0.00 |
| ATOM | 1217 CG | ARG | S | 523 | 38.180 | 48.804 | 30.091 | 1.00 | 0.00 |
| ATOM | 1218 CD | ARG | S | 523 | 37.008 | 49.394 | 29.317 | 1.00 | 0.00 |
| ATOM | 1219 NE | ARG | S | 523 | 35.768 | 48.936 | 29.939 | 1.00 | 0.00 |
| ATOM | 1220 CZ | ARG | S | 523 | 34.752 | 49.798 | 30.149 | 1.00 | 0.00 |
| ATOM | 1221 NH1 | ARG | S | 523 | 34.808 | 51.047 | 29.702 | 1.00 | 0.00 |
| ATOM | 1222 NH2 | ARG | S | 523 | 33.672 | 49.374 | 30.799 | 1.00 | 0.00 |
| ATOM | 1223 H | ARG | S | 523 | 39.672 | 49.608 | 32.512 | 1.00 | 0.00 |
| ATOM | 1224 HE | ARG | S | 523 | 35.690 | 47.988 | 30.260 | 1.00 | 0.00 |
| ATOM | 1225 1HH1 | ARG | S | 523 | 34.036 | 51.669 | 29.816 | 1.00 | 0.00 |
| ATOM | 1226 2HH1 | ARG | S | 523 | 35.608 | 51.442 | 29.256 | 1.00 | 0.00 |
| ATOM | 1227 1HH2 | ARG | S | 523 | 32.969 | 50.145 | 31.042 | 1.00 | 0.00 |
| ATOM | 1228 2HH2 | ARG | S | 523 | 33.535 | 48.419 | 31.065 | 1.00 | 0.00 |
| ATOM | 1229 N | ALA | S | 524 | 42.220 | 50.580 | 30.756 | 1.00 | 0.00 |
| ATOM | 1230 CA | ALA | S | 524 | 43.587 | 51.111 | 30.626 | 1.00 | 0.00 |
| ATOM | 1231 C | ALA | S | 524 | 44.744 | 50.245 | 31.144 | 1.00 | 0.00 |
| ATOM | 1232 O | ALA | S | 524 | 45.847 | 50.288 | 30.610 | 1.00 | 0.00 |
| ATOM | 1233 CB | ALA | S | 524 | 43.689 | 52.505 | 31.249 | 1.00 | 0.00 |
| ATOM | 1234 H | ALA | S | 524 | 41.473 | 51.161 | 31.073 | 1.00 | 0.00 |
| ATOM | 1235 N | GLN | S | 525 | 44.416 | 49.407 | 32.144 | 1.00 | 0.00 |
| ATOM | 1236 CA | GLN | S | 525 | 45.237 | 48.275 | 32.570 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1237 C | GLN | S | 525 | 45.326 | 47.166 | 31.521 | 1.00 | 0.00 |
| ATOM | 1238 O | GLN | S | 525 | 46.327 | 47.068 | 30.813 | 1.00 | 0.00 |
| ATOM | 1239 CB | GLN | S | 525 | 44.736 | 47.773 | 33.933 | 1.00 | 0.00 |
| ATOM | 1240 CG | GLN | S | 525 | 44.899 | 48.831 | 35.033 | 1.00 | 0.00 |
| ATOM | 1241 CD | GLN | S | 525 | 43.978 | 48.563 | 36.213 | 1.00 | 0.00 |
| ATOM | 1242 OE1 | GLN | S | 525 | 43.282 | 47.555 | 36.314 | 1.00 | 0.00 |
| ATOM | 1243 NE2 | GLN | S | 525 | 46.001 | 49.533 | 37.133 | 1.00 | 0.00 |
| ATOM | 1244 H | GLN | S | 525 | 43.464 | 49.490 | 32.435 | 1.00 | 0.00 |
| ATOM | 1245 1HE2 | GLN | S | 525 | 43.393 | 49.444 | 37.924 | 1.00 | 0.00 |
| ATOM | 1246 2HE2 | GLN | S | 525 | 44.621 | 50.307 | 37.028 | 1.00 | 0.00 |
| ATOM | 1247 N | TYR | S | 526 | 44.271 | 46.342 | 31.411 | 1.00 | 0.00 |
| ATOM | 1248 CA | TYR | S | 526 | 44.397 | 45.176 | 30.528 | 1.00 | 0.00 |
| ATOM | 1249 C | TYR | S | 526 | 44.513 | 45.432 | 29.024 | 1.00 | 0.00 |
| ATOM | 1250 O | TYR | S | 526 | 45.223 | 44.753 | 28.286 | 1.00 | 0.00 |
| ATOM | 1251 CB | TYR | S | 526 | 43.263 | 44.187 | 30.824 | 1.00 | 0.00 |
| ATOM | 1252 CG | TYR | S | 526 | 43.736 | 42.746 | 30.894 | 1.00 | 0.00 |
| ATOM | 1253 CD1 | TYR | S | 526 | 42.751 | 41.739 | 30.902 | 1.00 | 0.00 |
| ATOM | 1254 CD2 | TYR | S | 526 | 45.112 | 42.431 | 30.979 | 1.00 | 0.00 |
| ATOM | 1255 CE1 | TYR | S | 526 | 43.138 | 40.398 | 31.053 | 1.00 | 0.00 |
| ATOM | 1256 CE2 | TYR | S | 526 | 45.503 | 41.091 | 31.124 | 1.00 | 0.00 |
| ATOM | 1257 CZ | TYR | S | 526 | 44.508 | 40.096 | 31.180 | 1.00 | 0.00 |
| ATOM | 1258 OH | TYR | S | 526 | 44.892 | 38.780 | 31.363 | 1.00 | 0.00 |
| ATOM | 1259 H | TYR | S | 526 | 43.457 | 46.506 | 31.971 | 1.00 | 0.00 |
| ATOM | 1260 HH | TYR | S | 526 | 44.780 | 38.404 | 30.487 | 1.00 | 0.00 |
| ATOM | 1261 N | ILE | S | 527 | 43.739 | 46.442 | 28.603 | 1.00 | 0.00 |
| ATOM | 1262 CA | ILE | S | 527 | 43.698 | 46.928 | 27.220 | 1.00 | 0.00 |
| ATOM | 1263 C | ILE | S | 527 | 43.973 | 48.433 | 27.181 | 1.00 | 0.00 |
| ATOM | 1264 O | ILE | S | 527 | 44.330 | 49.028 | 28.197 | 1.00 | 0.00 |
| ATOM | 1265 CB | ILE | S | 527 | 42.360 | 46.549 | 26.566 | 1.00 | 0.00 |
| ATOM | 1266 CG1 | ILE | S | 527 | 41.195 | 46.911 | 27.490 | 1.00 | 0.00 |
| ATOM | 1267 CG2 | ILE | S | 527 | 42.359 | 45.050 | 26.242 | 1.00 | 0.00 |
| ATOM | 1268 CD1 | ILE | S | 527 | 39.829 | 46.475 | 26.968 | 1.00 | 0.00 |
| ATOM | 1269 H | ILE | S | 527 | 43.188 | 46.902 | 29.294 | 1.00 | 0.00 |
| ATOM | 1270 N | GLU | S | 528 | 43.854 | 49.037 | 25.998 | 1.00 | 0.00 |
| ATOM | 1271 CA | GLU | S | 528 | 44.150 | 50.461 | 25.901 | 1.00 | 0.00 |
| ATOM | 1272 C | GLU | S | 528 | 43.247 | 51.168 | 24.898 | 1.00 | 0.00 |
| ATOM | 1273 O | GLU | S | 528 | 42.828 | 50.587 | 23.896 | 1.00 | 0.00 |
| ATOM | 1274 CB | GLU | S | 528 | 45.625 | 50.638 | 25.559 | 1.00 | 0.00 |
| ATOM | 1275 CG | GLU | S | 528 | 46.353 | 51.685 | 26.418 | 1.00 | 0.00 |
| ATOM | 1276 CD | GLU | S | 528 | 45.696 | 53.031 | 26.214 | 1.00 | 0.00 |
| ATOM | 1277 OE1 | GLU | S | 528 | 44.958 | 53.471 | 27.084 | 1.00 | 0.00 |
| ATOM | 1278 OE2 | GLU | S | 528 | 45.880 | 53.627 | 25.159 | 1.00 | 0.00 |
| ATOM | 1279 H | GLU | S | 528 | 43.558 | 48.513 | 25.202 | 1.00 | 0.00 |
| ATOM | 1280 N | PHE | S | 529 | 42.943 | 52.442 | 25.200 | 1.00 | 0.00 |
| ATOM | 1281 CA | PHE | S | 529 | 42.027 | 53.226 | 24.362 | 1.00 | 0.00 |
| ATOM | 1282 C | PHE | S | 529 | 42.594 | 54.578 | 23.924 | 1.00 | 0.00 |
| ATOM | 1283 O | PHE | S | 529 | 43.746 | 54.632 | 23.481 | 1.00 | 0.00 |
| ATOM | 1284 CB | PHE | S | 529 | 40.641 | 53.291 | 25.025 | 1.00 | 0.00 |
| ATOM | 1285 CG | PHE | S | 529 | 40.018 | 51.918 | 24.964 | 1.00 | 0.00 |
| ATOM | 1286 CD1 | PHE | S | 529 | 40.028 | 51.101 | 26.114 | 1.00 | 0.00 |
| ATOM | 1287 CD2 | PHE | S | 529 | 39.467 | 51.463 | 23.746 | 1.00 | 0.00 |
| ATOM | 1288 CE1 | PHE | S | 529 | 39.521 | 49.792 | 26.028 | 1.00 | 0.00 |
| ATOM | 1289 CE2 | PHE | S | 529 | 38.962 | 50.153 | 23.661 | 1.00 | 0.00 |
| ATOM | 1290 CZ | PHE | S | 529 | 39.013 | 49.323 | 24.798 | 1.00 | 0.00 |
| ATOM | 1291 H | PHE | S | 529 | 43.379 | 52.870 | 25.995 | 1.00 | 0.00 |
| ATOM | 1292 N | SER | S | 530 | 41.814 | 55.664 | 24.049 | 1.00 | 0.00 |
| ATOM | 1293 CA | SER | S | 530 | 42.301 | 56.984 | 23.518 | 1.00 | 0.00 |
| ATOM | 1294 C | SER | S | 530 | 41.809 | 58.113 | 24.321 | 1.00 | 0.00 |
| ATOM | 1295 O | SER | S | 530 | 40.727 | 58.104 | 24.905 | 1.00 | 0.00 |
| ATOM | 1296 CB | SER | S | 530 | 41.853 | 57.145 | 22.075 | 1.00 | 0.00 |
| ATOM | 1297 OG | SER | S | 530 | 42.555 | 56.289 | 21.156 | 1.00 | 0.00 |
| ATOM | 1298 H | SER | S | 530 | 40.883 | 55.600 | 24.391 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1299 HG | SER | S | 530 | 42.517 | 56.792 | 20.347 | 1.00 | 0.00 |
| ATOM | 1300 N | LYS | S | 531 | 42.663 | 59.151 | 24.339 | 1.00 | 0.00 |
| ATOM | 1301 CA | LYS | S | 531 | 42.189 | 60.389 | 24.943 | 1.00 | 0.00 |
| ATOM | 1302 C | LYS | S | 531 | 41.774 | 61.528 | 24.019 | 1.00 | 0.00 |
| ATOM | 1303 O | LYS | S | 531 | 40.713 | 62.085 | 24.263 | 1.00 | 0.00 |
| ATOM | 1304 CB | LYS | S | 531 | 43.070 | 60.858 | 26.111 | 1.00 | 0.00 |
| ATOM | 1305 CG | LYS | S | 531 | 42.361 | 61.058 | 27.470 | 1.00 | 0.00 |
| ATOM | 1306 CD | LYS | S | 531 | 41.487 | 62.311 | 27.687 | 1.00 | 0.00 |
| ATOM | 1307 CE | LYS | S | 531 | 40.019 | 62.235 | 27.238 | 1.00 | 0.00 |
| ATOM | 1308 NZ | LYS | S | 531 | 39.316 | 63.464 | 27.624 | 1.00 | 0.00 |
| ATOM | 1309 H | LYS | S | 531 | 43.507 | 59.140 | 23.800 | 1.00 | 0.00 |
| ATOM | 1310 1HZ | LYS | S | 531 | 38.343 | 63.428 | 27.271 | 1.00 | 0.00 |
| ATOM | 1311 2HZ | LYS | S | 531 | 39.247 | 63.600 | 28.657 | 1.00 | 0.00 |
| ATOM | 1312 3HZ | LYS | S | 531 | 39.795 | 64.281 | 27.210 | 1.00 | 0.00 |
| ATOM | 1313 N | PRO | S | 532 | 42.554 | 61.918 | 22.981 | 1.00 | 0.00 |
| ATOM | 1314 CA | PRO | S | 532 | 41.987 | 62.910 | 22.048 | 1.00 | 0.00 |
| ATOM | 1315 C | PRO | S | 532 | 41.125 | 62.297 | 20.940 | 1.00 | 0.00 |
| ATOM | 1316 O | PRO | S | 532 | 41.182 | 62.659 | 19.759 | 1.00 | 0.00 |
| ATOM | 1317 CB | PRO | S | 532 | 43.251 | 63.610 | 21.546 | 1.00 | 0.00 |
| ATOM | 1318 CG | PRO | S | 532 | 44.323 | 62.521 | 21.526 | 1.00 | 0.00 |
| ATOM | 1319 CD | PRO | S | 532 | 43.942 | 61.586 | 22.672 | 1.00 | 0.00 |
| ATOM | 1320 N | PHE | S | 533 | 40.317 | 61.296 | 21.346 | 1.00 | 0.00 |
| ATOM | 1321 CA | PHE | S | 533 | 39.401 | 60.803 | 20.322 | 1.00 | 0.00 |
| ATOM | 1322 C | PHE | S | 533 | 38.207 | 61.716 | 20.115 | 1.00 | 0.00 |
| ATOM | 1323 O | PHE | S | 533 | 38.250 | 62.661 | 19.330 | 1.00 | 0.00 |
| ATOM | 1324 CB | PHE | S | 533 | 39.005 | 59.331 | 20.560 | 1.00 | 0.00 |
| ATOM | 1325 CG | PHE | S | 533 | 38.109 | 58.800 | 19.542 | 1.00 | 0.00 |
| ATOM | 1326 CD1 | PHE | S | 533 | 36.900 | 58.161 | 19.803 | 1.00 | 0.00 |
| ATOM | 1327 CD2 | PHE | S | 533 | 38.479 | 58.950 | 18.094 | 1.00 | 0.00 |
| ATOM | 1328 CE1 | PHE | S | 533 | 36.050 | 57.669 | 18.795 | 1.00 | 0.00 |
| ATOM | 1329 CE2 | PHE | S | 533 | 37.630 | 58.459 | 17.083 | 1.00 | 0.00 |
| ATOM | 1330 CZ | PHE | S | 533 | 36.423 | 57.825 | 17.444 | 1.00 | 0.00 |
| ATOM | 1331 H | PHE | S | 533 | 40.157 | 61.205 | 22.327 | 1.00 | 0.00 |
| ATOM | 1332 N | LYS | S | 534 | 37.111 | 61.380 | 20.816 | 1.00 | 0.00 |
| ATOM | 1333 CA | LYS | S | 534 | 35.919 | 32.191 | 20.634 | 1.00 | 0.00 |
| ATOM | 1334 C | LYS | S | 534 | 35.958 | 63.348 | 21.607 | 1.00 | 0.00 |
| ATOM | 1335 O | LYS | S | 534 | 35.812 | 63.121 | 22.809 | 1.00 | 0.00 |
| ATOM | 1336 CB | LYS | S | 534 | 34.698 | 61.275 | 20.818 | 1.00 | 0.00 |
| ATOM | 1337 CG | LYS | S | 534 | 33.347 | 61.986 | 20.775 | 1.00 | 0.00 |
| ATOM | 1338 CD | LYS | S | 534 | 33.201 | 62.809 | 19.503 | 1.00 | 0.00 |
| ATOM | 1339 CE | LYS | S | 534 | 32.094 | 63.839 | 19.641 | 1.00 | 0.00 |
| ATOM | 1340 NZ | LYS | S | 534 | 32.370 | 64.947 | 18.736 | 1.00 | 0.00 |
| ATOM | 1341 H | LYS | S | 534 | 37.099 | 60.595 | 21.442 | 1.00 | 0.00 |
| ATOM | 1342 1HZ | LYS | S | 534 | 33.380 | 65.198 | 18.751 | 1.00 | 0.00 |
| ATOM | 1343 2HZ | LYS | S | 534 | 32.167 | 64.628 | 17.777 | 1.00 | 0.00 |
| ATOM | 1344 3HZ | LYS | S | 534 | 31.800 | 65.789 | 18.908 | 1.00 | 0.00 |
| ATOM | 1345 N | TYR | S | 535 | 36.213 | 64.537 | 21.039 | 1.00 | 0.00 |
| ATOM | 1346 CA | TYR | S | 535 | 36.138 | 65.804 | 21.773 | 1.00 | 0.00 |
| ATOM | 1347 C | TYR | S | 535 | 36.295 | 65.779 | 23.303 | 1.00 | 0.00 |
| ATOM | 1348 O | TYR | S | 535 | 37.391 | 65.841 | 23.869 | 1.00 | 0.00 |
| ATOM | 1349 CB | TYR | S | 535 | 34.809 | 66.548 | 21.271 | 1.00 | 0.00 |
| ATOM | 1350 CG | TYR | S | 535 | 35.095 | 68.045 | 21.266 | 1.00 | 0.00 |
| ATOM | 1351 CD1 | TYR | S | 535 | 36.159 | 68.605 | 20.526 | 1.00 | 0.00 |
| ATOM | 1352 CD2 | TYR | S | 535 | 34.200 | 68.842 | 22.003 | 1.00 | 0.00 |
| ATOM | 1353 CE1 | TYR | S | 535 | 36.352 | 69.996 | 20.555 | 1.00 | 0.00 |
| ATOM | 1354 CE2 | TYR | S | 535 | 34.393 | 70.231 | 20.025 | 1.00 | 0.00 |
| ATOM | 1355 CZ | TYR | S | 535 | 35.479 | 70.792 | 21.323 | 1.00 | 0.00 |
| ATOM | 1356 OH | TYR | S | 535 | 35.712 | 72.156 | 21.409 | 1.00 | 0.00 |
| ATOM | 1357 H | TYR | S | 535 | 36.422 | 64.539 | 20.060 | 1.00 | 0.00 |
| ATOM | 1358 HH | TYR | S | 535 | 35.003 | 72.544 | 21.932 | 1.00 | 0.00 |
| ATOM | 1359 N | GLN | S | 536 | 35.154 | 65.689 | 24.015 | 1.00 | 0.00 |
| ATOM | 1360 CA | GLN | S | 536 | 35.198 | 65.687 | 25.488 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1361 C | GLN | S | 536 | 34.272 | 64.623 | 26.067 | 1.00 | 0.00 |
| ATOM | 1362 O | GLN | S | 536 | 33.306 | 64.240 | 25.405 | 1.00 | 0.00 |
| ATOM | 1363 CB | GLN | S | 536 | 34.736 | 67.045 | 26.032 | 1.00 | 0.00 |
| ATOM | 1364 CG | GLN | S | 536 | 35.484 | 68.275 | 25.306 | 1.00 | 0.00 |
| ATOM | 1365 CD | GLN | S | 536 | 34.792 | 69.532 | 25.996 | 1.00 | 0.00 |
| ATOM | 1366 OE1 | GLN | S | 536 | 34.000 | 69.529 | 26.937 | 1.00 | 0.00 |
| ATOM | 1367 NE2 | GLN | S | 536 | 35.120 | 70.641 | 25.332 | 1.00 | 0.00 |
| ATOM | 1368 H | GLN | S | 536 | 34.282 | 65.547 | 23.543 | 1.00 | 0.00 |
| ATOM | 1369 1HE2 | GLN | S | 536 | 34.658 | 71.515 | 25.490 | 1.00 | 0.00 |
| ATOM | 1370 2HE2 | GLN | S | 536 | 35.798 | 70.598 | 24.601 | 1.00 | 0.00 |
| ATOM | 1371 N | GLY | S | 537 | 34.523 | 64.191 | 27.323 | 1.00 | 0.00 |
| ATOM | 1372 CA | GLY | S | 537 | 33.513 | 63.349 | 27.992 | 1.00 | 0.00 |
| ATOM | 1373 C | GLY | S | 537 | 33.575 | 63.366 | 29.519 | 1.00 | 0.00 |
| ATOM | 1374 O | GLY | S | 537 | 34.373 | 62.671 | 30.158 | 1.00 | 0.00 |
| ATOM | 1375 H | GLY | S | 537 | 35.371 | 64.450 | 27.781 | 1.00 | 0.00 |
| ATOM | 1376 N | LEU | S | 538 | 32.734 | 64.246 | 30.087 | 1.00 | 0.00 |
| ATOM | 1377 CA | LEU | S | 538 | 32.935 | 64.570 | 31.497 | 1.00 | 0.00 |
| ATOM | 1378 C | LEU | S | 538 | 31.743 | 64.293 | 32.397 | 1.00 | 0.00 |
| ATOM | 1379 O | LEU | S | 538 | 30.647 | 63.918 | 31.969 | 1.00 | 0.00 |
| ATOM | 1380 CB | LEU | S | 538 | 33.417 | 66.021 | 31.640 | 1.00 | 0.00 |
| ATOM | 1381 CG | LEU | S | 538 | 34.934 | 66.213 | 31.621 | 1.00 | 0.00 |
| ATOM | 1382 CD1 | LEU | S | 538 | 35.600 | 65.240 | 32.585 | 1.00 | 0.00 |
| ATOM | 1383 CD2 | LEU | S | 538 | 35.554 | 66.173 | 30.224 | 1.00 | 0.00 |
| ATOM | 1384 H | LEU | S | 538 | 32.075 | 64.788 | 29.570 | 1.00 | 0.00 |
| ATOM | 1385 N | THR | S | 539 | 32.030 | 64.465 | 33.701 | 1.00 | 0.00 |
| ATOM | 1386 CA | THR | S | 539 | 31.038 | 64.027 | 34.676 | 1.00 | 0.00 |
| ATOM | 1387 C | THR | S | 539 | 29.992 | 65.072 | 35.029 | 1.00 | 0.00 |
| ATOM | 1388 O | THR | S | 539 | 30.280 | 66.230 | 35.334 | 1.00 | 0.00 |
| ATOM | 1389 CB | THR | S | 539 | 31.740 | 63.452 | 35.913 | 1.00 | 0.00 |
| ATOM | 1390 OG1 | THR | S | 539 | 32.950 | 63.775 | 35.522 | 1.00 | 0.00 |
| ATOM | 1391 CG2 | THR | S | 539 | 30.848 | 62.447 | 36.642 | 1.00 | 0.00 |
| ATOM | 1392 H | THR | S | 539 | 32.798 | 65.061 | 33.932 | 1.00 | 0.00 |
| ATOM | 1393 HG1 | THR | S | 539 | 33.585 | 63.450 | 35.257 | 1.00 | 0.00 |
| ATOM | 1394 N | ILE | S | 540 | 28.742 | 64.585 | 34.939 | 1.00 | 0.00 |
| ATOM | 1395 CA | ILE | S | 540 | 27.622 | 65.497 | 34.754 | 1.00 | 0.00 |
| ATOM | 1396 C | ILE | S | 540 | 26.944 | 66.158 | 35.961 | 1.00 | 0.00 |
| ATOM | 1397 O | ILE | S | 540 | 26.404 | 65.548 | 36.899 | 1.00 | 0.00 |
| ATOM | 1398 CB | ILE | S | 540 | 26.665 | 64.802 | 33.767 | 1.00 | 0.00 |
| ATOM | 1399 CG1 | ILE | S | 540 | 26.036 | 65.745 | 32.758 | 1.00 | 0.00 |
| ATOM | 1400 CG2 | ILE | S | 540 | 25.607 | 63.955 | 34.463 | 1.00 | 0.00 |
| ATOM | 1401 CD1 | ILE | S | 540 | 26.971 | 65.932 | 31.568 | 1.00 | 0.00 |
| ATOM | 1402 H | ILE | S | 540 | 28.599 | 63.617 | 34.765 | 1.00 | 0.00 |
| ATOM | 1403 N | LEU | S | 541 | 26.982 | 67.482 | 35.864 | 1.00 | 0.00 |
| ATOM | 1404 CA | LEU | S | 541 | 26.266 | 68.353 | 36.782 | 1.00 | 0.00 |
| ATOM | 1405 C | LEU | S | 541 | 24.836 | 68.705 | 36.423 | 1.00 | 0.00 |
| ATOM | 1406 O | LEU | S | 541 | 24.290 | 69.690 | 36.912 | 1.00 | 0.00 |
| ATOM | 1407 CB | LEU | S | 541 | 27.035 | 69.647 | 36.999 | 1.00 | 0.00 |
| ATOM | 1408 CG | LEU | S | 541 | 27.872 | 69.601 | 38.267 | 1.00 | 0.00 |
| ATOM | 1409 CD1 | LEU | S | 541 | 29.126 | 68.738 | 38.121 | 1.00 | 0.00 |
| ATOM | 1410 CD2 | LEU | S | 541 | 28.146 | 71.011 | 38.768 | 1.00 | 0.00 |
| ATOM | 1411 H | LEU | S | 541 | 27.559 | 67.836 | 35.140 | 1.00 | 0.00 |
| ATOM | 1412 N | VAL | S | 542 | 24.204 | 67.886 | 35.577 | 1.00 | 0.00 |
| ATOM | 1413 CA | VAL | S | 542 | 22.775 | 68.138 | 35.328 | 1.00 | 0.00 |
| ATOM | 1414 C | VAL | S | 542 | 21.892 | 68.030 | 36.567 | 1.00 | 0.00 |
| ATOM | 1415 O | VAL | S | 542 | 22.281 | 67.388 | 37.549 | 1.00 | 0.00 |
| ATOM | 1416 CB | VAL | S | 542 | 22.244 | 67.183 | 34.269 | 1.00 | 0.00 |
| ATOM | 1417 CG1 | VAL | S | 542 | 22.818 | 67.490 | 32.886 | 1.00 | 0.00 |
| ATOM | 1418 CG2 | VAL | S | 542 | 22.439 | 65.735 | 34.728 | 1.00 | 0.00 |
| ATOM | 1419 H | VAL | S | 542 | 24.787 | 67.195 | 35.153 | 1.00 | 0.00 |
| ATOM | 1420 N | LYS | S | 543 | 20.673 | 68.617 | 36.430 | 1.00 | 0.00 |
| ATOM | 1421 CA | LYS | S | 543 | 19.558 | 68.746 | 37.391 | 1.00 | 0.00 |
| ATOM | 1422 C | LYS | S | 543 | 19.435 | 70.138 | 37.995 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1423 O | LYS | S | 543 | 20.126 | 70.433 | 38.960 | 1.00 | 0.00 |
| ATOM | 1424 CB | LYS | S | 543 | 19.575 | 67.732 | 38.553 | 1.00 | 0.00 |
| ATOM | 1425 CG | LYS | S | 543 | 18.383 | 67.813 | 39.515 | 1.00 | 0.00 |
| ATOM | 1426 CD | LYS | S | 543 | 18.788 | 67.755 | 40.994 | 1.00 | 0.00 |
| ATOM | 1427 CE | LYS | S | 543 | 19.480 | 69.303 | 41.480 | 1.00 | 0.00 |
| ATOM | 1428 NZ | LYS | S | 543 | 20.222 | 68.779 | 42.712 | 1.00 | 0.00 |
| ATOM | 1429 H | LYS | S | 543 | 20.531 | 69.102 | 35.556 | 1.00 | 0.00 |
| ATOM | 1430 1HZ | LYS | S | 543 | 19.746 | 68.943 | 43.618 | 1.00 | 0.00 |
| ATOM | 1431 2HZ | LYS | S | 543 | 20.541 | 67.800 | 42.677 | 1.00 | 0.00 |
| ATOM | 1432 3HZ | LYS | S | 543 | 21.101 | 69.332 | 42.764 | 1.00 | 0.00 |
| ATOM | 1433 N | LYS | S | 544 | 18.500 | 70.954 | 37.456 | 1.00 | 0.00 |
| ATOM | 1434 CA | LYS | S | 544 | 18.289 | 72.317 | 37.987 | 1.00 | 0.00 |
| ATOM | 1435 C | LYS | S | 544 | 19.534 | 73.179 | 37.827 | 1.00 | 0.00 |
| ATOM | 1436 O | LYS | S | 544 | 20.575 | 72.927 | 38.427 | 1.00 | 0.00 |
| ATOM | 1437 CB | LYS | S | 544 | 17.758 | 72.344 | 39.435 | 1.00 | 0.00 |
| ATOM | 1438 CG | LYS | S | 544 | 16.771 | 71.226 | 39.806 | 1.00 | 0.00 |
| ATOM | 1439 CD | LYS | S | 544 | 15.485 | 71.170 | 38.982 | 1.00 | 0.00 |
| ATOM | 1440 CE | LYS | S | 544 | 14.650 | 69.919 | 39.280 | 1.00 | 0.00 |
| ATOM | 1441 NZ | LYS | S | 544 | 15.233 | 68.714 | 38.685 | 1.00 | 0.00 |
| ATOM | 1442 H | LYS | S | 544 | 18.346 | 70.792 | 36.479 | 1.00 | 0.00 |
| ATOM | 1443 1HZ | LYS | S | 544 | 14.510 | 68.232 | 38.127 | 1.00 | 0.00 |
| ATOM | 1444 2HZ | LYS | S | 544 | 16.029 | 68.936 | 38.064 | 1.00 | 0.00 |
| ATOM | 1445 3HZ | LYS | S | 544 | 15.549 | 68.078 | 39.440 | 1.00 | 0.00 |
| ATOM | 1446 N | GLU | S | 545 | 19.410 | 74.104 | 36.879 | 1.00 | 0.00 |
| ATOM | 1447 CA | GLU | S | 545 | 20.636 | 74.523 | 36.214 | 1.00 | 0.00 |
| ATOM | 1448 C | GLU | S | 545 | 20.732 | 76.054 | 36.116 | 1.00 | 0.00 |
| ATOM | 1449 O | GLU | S | 545 | 19.868 | 76.776 | 36.623 | 1.00 | 0.00 |
| ATOM | 1450 CB | GLU | S | 545 | 20.750 | 73.690 | 34.909 | 1.00 | 0.00 |
| ATOM | 1451 CG | GLU | S | 545 | 21.054 | 72.183 | 35.134 | 1.00 | 0.00 |
| ATOM | 1452 CD | GLU | S | 545 | 20.209 | 71.203 | 34.302 | 1.00 | 0.00 |
| ATOM | 1453 OE1 | GLU | S | 545 | 19.213 | 70.663 | 34.778 | 1.00 | 0.00 |
| ATOM | 1454 OE2 | GLU | S | 545 | 20.557 | 70.909 | 33.172 | 1.00 | 0.00 |
| ATOM | 1455 H | GLU | S | 545 | 18.513 | 74.251 | 36.477 | 1.00 | 0.00 |
| ATOM | 1456 N | ILE | S | 546 | 21.858 | 76.538 | 35.532 | 1.00 | 0.00 |
| ATOM | 1457 CA | ILE | S | 546 | 22.274 | 77.935 | 35.757 | 1.00 | 0.00 |
| ATOM | 1458 C | ILE | S | 546 | 21.234 | 78.998 | 35.420 | 1.00 | 0.00 |
| ATOM | 1459 O | ILE | S | 546 | 20.724 | 79.133 | 34.310 | 1.00 | 0.00 |
| ATOM | 1460 CB | ILE | S | 546 | 23.632 | 78.256 | 35.082 | 1.00 | 0.00 |
| ATOM | 1461 CG1 | ILE | S | 546 | 24.759 | 77.346 | 35.573 | 1.00 | 0.00 |
| ATOM | 1462 CG2 | ILE | S | 546 | 24.065 | 79.718 | 35.275 | 1.00 | 0.00 |
| ATOM | 1463 CD1 | ILE | S | 546 | 26.069 | 77.508 | 34.796 | 1.00 | 0.00 |
| ATOM | 1464 H | ILE | S | 546 | 22.453 | 75.915 | 35.013 | 1.00 | 0.00 |
| ATOM | 1465 N | PRO | S | 547 | 20.906 | 79.788 | 36.469 | 1.00 | 0.00 |
| ATOM | 1466 CA | PRO | S | 547 | 20.093 | 80.981 | 36.235 | 1.00 | 0.00 |
| ATOM | 1467 C | PRO | S | 547 | 20.897 | 82.045 | 35.497 | 1.00 | 0.00 |
| ATOM | 1468 O | PRO | S | 547 | 21.711 | 82.774 | 36.068 | 1.00 | 0.00 |
| ATOM | 1469 CB | PRO | S | 547 | 19.690 | 81.372 | 27.661 | 1.00 | 0.00 |
| ATOM | 1470 CG | PRO | S | 547 | 20.840 | 80.904 | 38.553 | 1.00 | 0.00 |
| ATOM | 1471 CD | PRO | S | 547 | 21.308 | 79.630 | 37.863 | 1.00 | 0.00 |
| ATOM | 1472 N | ARG | S | 548 | 20.612 | 82.072 | 34.199 | 1.00 | 0.00 |
| ATOM | 1473 CA | ARG | S | 548 | 21.224 | 83.027 | 33.295 | 1.00 | 0.00 |
| ATOM | 1474 C | ARG | S | 548 | 20.135 | 83.812 | 32.555 | 1.00 | 0.00 |
| ATOM | 1475 O | ARG | S | 548 | 19.020 | 83.927 | 33.065 | 1.00 | 0.00 |
| ATOM | 1476 CB | ARG | S | 548 | 22.264 | 82.286 | 32.404 | 1.00 | 0.00 |
| ATOM | 1477 CG | ARG | S | 548 | 21.946 | 81.675 | 31.012 | 1.00 | 0.00 |
| ATOM | 1478 CD | ARG | S | 548 | 20.809 | 80.650 | 30.871 | 1.00 | 0.00 |
| ATOM | 1479 NE | ARG | S | 548 | 19.546 | 81.274 | 31.228 | 1.00 | 0.00 |
| ATOM | 1480 CZ | ARG | S | 548 | 18.673 | 80.636 | 32.017 | 1.00 | 0.00 |
| ATOM | 1481 NH1 | ARG | S | 548 | 17.913 | 81.352 | 32.824 | 1.00 | 0.00 |
| ATOM | 1482 NH2 | ARG | S | 548 | 18.858 | 79.321 | 32.022 | 1.00 | 0.00 |
| ATOM | 1483 OXT | ARG | S | 548 | 20.357 | 84.258 | 31.430 | 1.00 | 0.00 |
| ATOM | 1484 H | ARG | S | 548 | 19.972 | 81.699 | 33.843 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1485 HE | ARG | S | 548 | 19.512 | 82.274 | 31.155 | 1.00 | 0.00 |
| ATOM | 1486 1HH1 | ARG | S | 548 | 17.211 | 80.913 | 33.383 | 1.00 | 0.00 |
| ATOM | 1487 2HH1 | ARG | S | 548 | 18.085 | 82.343 | 32.896 | 1.00 | 0.00 |
| ATOM | 1488 1HH2 | ARG | S | 548 | 17.943 | 78.877 | 32.638 | 1.00 | 0.00 |
| ATOM | 1489 2HH2 | ARG | S | 548 | 19.157 | 78.764 | 31.415 | 1.00 | 0.00 |
| ATOM | 1490 N | PRO | S | 660 | 4.523 | 80.852 | 31.091 | 1.00 | 0.00 |
| ATOM | 1491 CA | PRO | S | 660 | 5.011 | 81.934 | 30.221 | 1.00 | 0.00 |
| ATOM | 1492 C | PRO | S | 660 | 5.983 | 82.768 | 31.022 | 1.00 | 0.00 |
| ATOM | 1493 O | PRO | S | 660 | 5.582 | 83.600 | 31.825 | 1.00 | 0.00 |
| ATOM | 1494 CB | PRO | S | 660 | 3.784 | 82.712 | 29.738 | 1.00 | 0.00 |
| ATOM | 1495 CG | PRO | S | 660 | 2.638 | 82.135 | 30.563 | 1.00 | 0.00 |
| ATOM | 1496 CD | PRO | S | 660 | 3.090 | 80.705 | 30.840 | 1.00 | 0.00 |
| ATOM | 1497 1H | PRO | S | 660 | 4.695 | 81.128 | 32.081 | 1.00 | 0.00 |
| ATOM | 1498 2H | PRO | S | 660 | 5.080 | 79.971 | 30.998 | 1.00 | 0.00 |
| ATOM | 1499 N | GLU | S | 661 | 7.260 | 82.412 | 30.806 | 1.00 | 0.00 |
| ATOM | 1500 CA | GLU | S | 661 | 8.328 | 82.728 | 31.747 | 1.00 | 0.00 |
| ATOM | 1501 C | GLU | S | 661 | 9.637 | 82.842 | 31.000 | 1.00 | 0.00 |
| ATOM | 1502 O | GLU | S | 661 | 10.032 | 81.902 | 30.801 | 1.00 | 0.00 |
| ATOM | 1503 CB | GLU | S | 661 | 8.603 | 81.578 | 32.735 | 1.00 | 0.00 |
| ATOM | 1504 CG | GLU | S | 661 | 7.484 | 80.687 | 33.297 | 1.00 | 0.00 |
| ATOM | 1505 CD | GLU | S | 661 | 6.800 | 79.788 | 32.266 | 1.00 | 0.00 |
| ATOM | 1506 OE1 | GLU | S | 661 | 7.183 | 79.697 | 31.102 | 1.00 | 0.00 |
| ATOM | 1507 OE2 | GLU | S | 661 | 5.786 | 79.207 | 32.603 | 1.00 | 0.00 |
| ATOM | 1508 H | GLU | S | 661 | 7.509 | 81.749 | 30.100 | 1.00 | 0.00 |
| ATOM | 1509 N | GLU | S | 662 | 10.331 | 83.960 | 31.249 | 1.00 | 0.00 |
| ATOM | 1510 CA | GLU | S | 662 | 11.784 | 83.945 | 31.068 | 1.00 | 0.00 |
| ATOM | 1511 C | GLU | S | 662 | 12.393 | 82.710 | 31.703 | 1.00 | 0.00 |
| ATOM | 1512 O | GLU | S | 662 | 11.875 | 82.126 | 32.649 | 1.00 | 0.00 |
| ATOM | 1513 CB | GLU | S | 662 | 12.420 | 85.188 | 31.701 | 1.00 | 0.00 |
| ATOM | 1514 CG | GLU | S | 662 | 12.325 | 86.477 | 30.877 | 1.00 | 0.00 |
| ATOM | 1515 CD | GLU | S | 662 | 10.886 | 86.801 | 30.527 | 1.00 | 0.00 |
| ATOM | 1516 OE1 | GLU | S | 662 | 10.086 | 87.049 | 31.428 | 1.00 | 0.00 |
| ATOM | 1517 OE2 | GLU | S | 662 | 10.562 | 86.789 | 29.345 | 1.00 | 0.00 |
| ATOM | 1518 H | GLU | S | 662 | 9.908 | 84.826 | 31.534 | 1.00 | 0.00 |
| ATOM | 1519 N | ARG | S | 663 | 13.525 | 82.272 | 31.145 | 1.00 | 0.00 |
| ATOM | 1520 CA | ARG | S | 663 | 13.990 | 80.955 | 31.599 | 1.00 | 0.00 |
| ATOM | 1521 C | ARG | S | 663 | 14.688 | 80.893 | 32.960 | 1.00 | 0.00 |
| ATOM | 1522 O | ARG | S | 663 | 15.560 | 80.055 | 33.187 | 1.00 | 0.00 |
| ATOM | 1523 CB | ARG | S | 663 | 14.868 | 80.307 | 30.532 | 1.00 | 0.00 |
| ATOM | 1524 CG | ARG | S | 663 | 14.264 | 80.480 | 29.114 | 1.00 | 0.00 |
| ATOM | 1525 CD | ARG | S | 663 | 13.133 | 79.155 | 28.940 | 1.00 | 0.00 |
| ATOM | 1526 NE | ARG | S | 663 | 11.869 | 79.605 | 29.525 | 1.00 | 0.00 |
| ATOM | 1527 CZ | ARG | S | 663 | 10.881 | 78.730 | 29.804 | 1.00 | 0.00 |
| ATOM | 1528 NH1 | ARG | S | 663 | 9.787 | 79.206 | 30.385 | 1.00 | 0.00 |
| ATOM | 1529 NH2 | ARG | S | 663 | 11.011 | 77.437 | 29.518 | 1.00 | 0.00 |
| ATOM | 1530 H | ARG | S | 663 | 13.950 | 82.832 | 30.431 | 1.00 | 0.00 |
| ATOM | 1531 HE | ARG | S | 663 | 11.700 | 80.582 | 29.683 | 1.00 | 0.00 |
| ATOM | 1532 1HH1 | ARG | S | 663 | 8.978 | 78.677 | 30.649 | 1.00 | 0.00 |
| ATOM | 1533 2HH1 | ARG | S | 663 | 9.749 | 80.188 | 30.588 | 1.00 | 0.00 |
| ATOM | 1534 1HH2 | ARG | S | 663 | 10.327 | 76.750 | 29.748 | 1.00 | 0.00 |
| ATOM | 1535 2HH2 | ARG | S | 663 | 11.822 | 77.061 | 29.050 | 1.00 | 0.00 |
| ATOM | 1536 N | ILE | S | 664 | 14.340 | 81.831 | 33.855 | 1.00 | 0.00 |
| ATOM | 1537 CA | ILE | S | 664 | 15.047 | 81.887 | 35.137 | 1.00 | 0.00 |
| ATOM | 1538 C | ILE | S | 664 | 14.248 | 81.163 | 36.211 | 1.00 | 0.00 |
| ATOM | 1539 O | ILE | S | 664 | 13.803 | 81.696 | 37.221 | 1.00 | 0.00 |
| ATOM | 1540 CB | ILE | S | 664 | 15.351 | 83.342 | 35.528 | 1.00 | 0.00 |
| ATOM | 1541 CG1 | ILE | S | 664 | 15.803 | 84.151 | 34.306 | 1.00 | 0.00 |
| ATOM | 1542 CG2 | ILE | S | 664 | 16.428 | 83.374 | 36.620 | 1.00 | 0.00 |
| ATOM | 1543 CD1 | ILE | S | 664 | 16.001 | 85.639 | 34.601 | 1.00 | 0.00 |
| ATOM | 1544 H | ILE | S | 664 | 13.495 | 82.346 | 33.722 | 1.00 | 0.00 |
| ATOM | 1545 N | THR | S | 665 | 14.026 | 79.894 | 35.883 | 1.00 | 0.00 |
| ATOM | 1546 CA | THR | S | 665 | 13.041 | 79.085 | 36.593 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1547 C | THR | S | 665 | 13.578 | 78.301 | 37.785 | 1.00 | 0.00 |
| ATOM | 1548 O | THR | S | 665 | 13.106 | 77.210 | 38.142 | 1.00 | 0.00 |
| ATOM | 1549 CB | THR | S | 665 | 12.408 | 78.184 | 35.534 | 1.00 | 0.00 |
| ATOM | 1550 OG1 | THR | S | 665 | 13.403 | 77.832 | 34.554 | 1.00 | 0.00 |
| ATOM | 1551 CG2 | THR | S | 665 | 11.246 | 78.895 | 34.836 | 1.00 | 0.00 |
| ATOM | 1552 H | THR | S | 665 | 14.459 | 79.500 | 35.074 | 1.00 | 0.00 |
| ATOM | 1553 HG1 | THR | S | 665 | 13.913 | 77.137 | 34.972 | 1.00 | 0.00 |
| ATOM | 1554 N | GLY | S | 666 | 14.634 | 78.869 | 38.383 | 1.00 | 0.00 |
| ATOM | 1555 CA | GLY | S | 666 | 15.262 | 78.155 | 39.488 | 1.00 | 0.00 |
| ATOM | 1556 C | GLY | S | 666 | 16.760 | 78.368 | 39.558 | 1.00 | 0.00 |
| ATOM | 1557 O | GLY | S | 666 | 17.291 | 79.440 | 39.259 | 1.00 | 0.00 |
| ATOM | 1558 H | GLY | S | 666 | 14.977 | 79.764 | 38.101 | 1.00 | 0.00 |
| ATOM | 1559 N | ILE | S | 667 | 17.430 | 77.279 | 39.977 | 1.00 | 0.00 |
| ATOM | 1560 CA | ILE | S | 667 | 18.847 | 77.460 | 40.306 | 1.00 | 0.00 |
| ATOM | 1561 C | ILE | S | 667 | 19.705 | 76.167 | 40.197 | 1.00 | 0.00 |
| ATOM | 1562 O | ILE | S | 667 | 19.390 | 75.077 | 40.682 | 1.00 | 0.00 |
| ATOM | 1563 CB | ILE | S | 667 | 18.984 | 78.113 | 41.689 | 1.00 | 0.00 |
| ATOM | 1564 CG1 | ILE | S | 667 | 20.415 | 78.559 | 42.015 | 1.00 | 0.00 |
| ATOM | 1565 CG2 | ILE | S | 667 | 18.405 | 77.229 | 42.804 | 1.00 | 0.00 |
| ATOM | 1566 CD1 | ILE | S | 667 | 20.514 | 79.388 | 43.290 | 1.00 | 0.00 |
| ATOM | 1567 H | ILE | S | 667 | 16.966 | 76.450 | 40.283 | 1.00 | 0.00 |
| ATOM | 1568 N | ASN | S | 668 | 20.863 | 76.453 | 39.583 | 1.00 | 0.00 |
| ATOM | 1569 CA | ASN | S | 668 | 22.022 | 75.571 | 39.450 | 1.00 | 0.00 |
| ATOM | 1570 C | ASN | S | 668 | 22.461 | 74.760 | 40.653 | 1.00 | 0.00 |
| ATOM | 1571 O | ASN | S | 668 | 22.668 | 75.237 | 41.770 | 1.00 | 0.00 |
| ATOM | 1572 CB | ASN | S | 668 | 23.219 | 76.390 | 38.954 | 1.00 | 0.00 |
| ATOM | 1573 CG | ASN | S | 668 | 24.382 | 75.495 | 38.564 | 1.00 | 0.00 |
| ATOM | 1574 OD1 | ASN | S | 668 | 25.451 | 75.495 | 39.184 | 1.00 | 0.00 |
| ATOM | 1575 ND2 | ASN | S | 668 | 24.140 | 74.731 | 37.494 | 1.00 | 0.00 |
| ATOM | 1576 H | ASN | S | 668 | 20.864 | 77.354 | 39.160 | 1.00 | 0.00 |
| ATOM | 1577 1HD2 | ASN | S | 668 | 24.851 | 74.193 | 37.051 | 1.00 | 0.00 |
| ATOM | 1578 2HD2 | ASN | S | 668 | 23.217 | 74.741 | 37.115 | 1.00 | 0.00 |
| ATOM | 1579 N | ASP | S | 669 | 22.711 | 73.494 | 40.315 | 1.00 | 0.00 |
| ATOM | 1580 CA | ASP | S | 669 | 23.577 | 72.615 | 41.099 | 1.00 | 0.00 |
| ATOM | 1581 C | ASP | S | 669 | 25.058 | 72.919 | 40.856 | 1.00 | 0.00 |
| ATOM | 1582 O | ASP | S | 669 | 25.492 | 72.974 | 39.700 | 1.00 | 0.00 |
| ATOM | 1583 CB | ASP | S | 669 | 23.241 | 71.194 | 40.678 | 1.00 | 0.00 |
| ATOM | 1584 CG | ASP | S | 669 | 23.444 | 70.226 | 41.814 | 1.00 | 0.00 |
| ATOM | 1585 OD1 | ASP | S | 669 | 22.640 | 69.322 | 41.944 | 1.00 | 0.00 |
| ATOM | 1586 OD2 | ASP | S | 669 | 24.401 | 70.338 | 42.561 | 1.00 | 0.00 |
| ATOM | 1587 H | ASP | S | 669 | 22.264 | 73.158 | 39.483 | 1.00 | 0.00 |
| ATOM | 1588 N | PRO | S | 670 | 25.808 | 73.237 | 41.952 | 1.00 | 0.00 |
| ATOM | 1589 CA | PRO | S | 670 | 27.180 | 73.786 | 41.859 | 1.00 | 0.00 |
| ATOM | 1590 C | PRO | S | 670 | 28.368 | 72.949 | 42.403 | 1.00 | 0.00 |
| ATOM | 1591 O | PRO | S | 670 | 28.466 | 72.594 | 43.583 | 1.00 | 0.00 |
| ATOM | 1592 CB | PRO | S | 670 | 26.972 | 75.062 | 42.673 | 1.00 | 0.00 |
| ATOM | 1593 CG | PRO | S | 670 | 26.054 | 74.641 | 43.833 | 1.00 | 0.00 |
| ATOM | 1594 CD | PRO | S | 670 | 25.267 | 73.444 | 43.291 | 1.00 | 0.00 |
| ATOM | 1595 N | ARG | S | 671 | 29.364 | 72.702 | 41.522 | 1.00 | 0.00 |
| ATOM | 1596 CA | ARG | S | 671 | 30.550 | 71.865 | 41.842 | 1.00 | 0.00 |
| ATOM | 1597 C | ARG | S | 671 | 31.567 | 72.224 | 42.958 | 1.00 | 0.00 |
| ATOM | 1598 O | ARG | S | 671 | 32.429 | 71.421 | 43.338 | 1.00 | 0.00 |
| ATOM | 1599 CB | ARG | S | 671 | 31.290 | 71.577 | 40.523 | 1.00 | 0.00 |
| ATOM | 1600 CG | ARG | S | 671 | 31.760 | 70.130 | 40.297 | 1.00 | 0.00 |
| ATOM | 1601 CD | ARG | S | 671 | 33.097 | 69.783 | 40.951 | 1.00 | 0.00 |
| ATOM | 1602 NE | ARG | S | 671 | 33.426 | 68.362 | 40.856 | 1.00 | 0.00 |
| ATOM | 1603 CZ | ARG | S | 671 | 33.270 | 67.556 | 41.926 | 1.00 | 0.00 |
| ATOM | 1604 NH1 | ARG | S | 671 | 33.688 | 66.298 | 41.880 | 1.00 | 0.00 |
| ATOM | 1605 NH2 | ARG | S | 671 | 32.724 | 68.030 | 43.045 | 1.00 | 0.00 |
| ATOM | 1606 H | ARG | S | 671 | 29.083 | 72.852 | 40.574 | 1.00 | 0.00 |
| ATOM | 1607 HE | ARG | S | 671 | 33.913 | 68.068 | 40.029 | 1.00 | 0.00 |
| ATOM | 1608 1HH1 | ARG | S | 671 | 33.562 | 65.701 | 42.677 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1609 2HH1 | ARG | S | 671 | 34.123 | 65.922 | 41.067 | 1.00 | 0.00 |
| ATOM | 1610 1HH2 | ARG | S | 671 | 32.780 | 67.475 | 43.881 | 1.00 | 0.00 |
| ATOM | 1611 2HH2 | ARG | S | 671 | 32.275 | 68.931 | 43.074 | 1.00 | 0.00 |
| ATOM | 1612 N | LEU | S | 672 | 31.498 | 73.465 | 43.452 | 1.00 | 0.00 |
| ATOM | 1613 CA | LEU | S | 672 | 32.586 | 73.945 | 44.316 | 1.00 | 0.00 |
| ATOM | 1614 C | LEU | S | 672 | 32.800 | 73.117 | 45.584 | 1.00 | 0.00 |
| ATOM | 1615 O | LEU | S | 672 | 31.857 | 72.669 | 46.226 | 1.00 | 0.00 |
| ATOM | 1616 CB | LEU | S | 672 | 32.345 | 75.422 | 44.650 | 1.00 | 0.00 |
| ATOM | 1617 CG | LEU | S | 672 | 33.497 | 76.129 | 45.374 | 1.00 | 0.00 |
| ATOM | 1618 CD1 | LEU | S | 672 | 34.750 | 76.232 | 44.503 | 1.00 | 0.00 |
| ATOM | 1619 CD2 | LEU | S | 672 | 33.066 | 77.485 | 45.933 | 1.00 | 0.00 |
| ATOM | 1620 H | LEU | S | 672 | 30.729 | 74.021 | 43.156 | 1.00 | 0.00 |
| ATOM | 1621 N | LYS | S | 673 | 34.073 | 72.931 | 45.971 | 1.00 | 0.00 |
| ATOM | 1622 CA | LYS | S | 673 | 34.294 | 72.047 | 47.122 | 1.00 | 0.00 |
| ATOM | 1623 C | LYS | S | 673 | 33.605 | 72.423 | 48.435 | 1.00 | 0.00 |
| ATOM | 1624 O | LYS | S | 673 | 33.530 | 71.623 | 49.353 | 1.00 | 0.00 |
| ATOM | 1625 CB | LYS | S | 673 | 35.791 | 71.759 | 47.354 | 1.00 | 0.00 |
| ATOM | 1626 CG | LYS | S | 673 | 36.085 | 70.401 | 48.032 | 1.00 | 0.00 |
| ATOM | 1627 CD | LYS | S | 673 | 37.572 | 70.169 | 48.347 | 1.00 | 0.00 |
| ATOM | 1628 CE | LYS | S | 673 | 37.943 | 68.757 | 48.845 | 1.00 | 0.00 |
| ATOM | 1629 NZ | LYS | S | 673 | 37.417 | 68.473 | 50.186 | 1.00 | 0.00 |
| ATOM | 1630 H | LYS | S | 673 | 34.802 | 73.218 | 45.354 | 1.00 | 0.00 |
| ATOM | 1631 1HZ | LYS | S | 673 | 36.393 | 68.638 | 50.244 | 1.00 | 0.00 |
| ATOM | 1632 2HZ | LYS | S | 673 | 37.556 | 67.469 | 50.421 | 1.00 | 0.00 |
| ATOM | 1633 3HZ | LYS | S | 673 | 37.855 | 69.040 | 50.933 | 1.00 | 0.00 |
| ATOM | 1634 N | ASN | S | 674 | 33.109 | 73.670 | 48.539 | 1.00 | 0.00 |
| ATOM | 1635 CA | ASN | S | 674 | 32.342 | 73.971 | 49.762 | 1.00 | 0.00 |
| ATOM | 1636 C | ASN | S | 674 | 30.937 | 73.350 | 49.820 | 1.00 | 0.00 |
| ATOM | 1637 O | ASN | S | 674 | 30.663 | 72.579 | 50.740 | 1.00 | 0.00 |
| ATOM | 1638 CB | ASN | S | 674 | 32.394 | 75.459 | 50.186 | 1.00 | 0.00 |
| ATOM | 1639 CG | ASN | S | 674 | 33.828 | 75.947 | 50.305 | 1.00 | 0.00 |
| ATOM | 1640 OD1 | ASN | S | 674 | 34.640 | 75.762 | 49.406 | 1.00 | 0.00 |
| ATOM | 1641 ND2 | ASN | S | 674 | 34.123 | 76.573 | 51.448 | 1.00 | 0.00 |
| ATOM | 1642 H | ASN | S | 674 | 33.223 | 74.333 | 47.794 | 1.00 | 0.00 |
| ATOM | 1643 1HD2 | ASN | S | 674 | 35.070 | 76.884 | 51.538 | 1.00 | 0.00 |
| ATOM | 1644 2HD2 | ASN | S | 674 | 33.487 | 76.795 | 52.186 | 1.00 | 0.00 |
| ATOM | 1645 N | PRO | S | 675 | 30.064 | 73.624 | 48.791 | 1.00 | 0.00 |
| ATOM | 1646 CA | PRO | S | 675 | 28.902 | 72.744 | 48.580 | 1.00 | 0.00 |
| ATOM | 1647 C | PRO | S | 675 | 29.227 | 71.253 | 48.548 | 1.00 | 0.00 |
| ATOM | 1648 O | PRO | S | 675 | 28.861 | 70.541 | 49.476 | 1.00 | 0.00 |
| ATOM | 1649 CB | PRO | S | 675 | 28.215 | 73.298 | 47.322 | 1.00 | 0.00 |
| ATOM | 1650 CG | PRO | S | 675 | 29.195 | 74.265 | 46.671 | 1.00 | 0.00 |
| ATOM | 1651 CD | PRO | S | 675 | 30.077 | 74.724 | 47.825 | 1.00 | 0.00 |
| ATOM | 1652 N | SER | S | 676 | 30.004 | 70.834 | 47.529 | 1.00 | 0.00 |
| ATOM | 1653 CA | SER | S | 676 | 30.509 | 69.453 | 47.419 | 1.00 | 0.00 |
| ATOM | 1654 C | SER | S | 676 | 30.790 | 68.652 | 48.690 | 1.00 | 0.00 |
| ATOM | 1655 O | SER | S | 676 | 30.402 | 67.487 | 48.845 | 1.00 | 0.00 |
| ATOM | 1656 CB | SER | S | 676 | 31.755 | 69.427 | 46.533 | 1.00 | 0.00 |
| ATOM | 1657 OG | SER | S | 676 | 31.494 | 70.139 | 45.315 | 1.00 | 0.00 |
| ATOM | 1658 H | SER | S | 676 | 30.177 | 71.436 | 46.731 | 1.00 | 0.00 |
| ATOM | 1659 HG | SER | S | 676 | 32.237 | 70.723 | 45.137 | 1.00 | 0.00 |
| ATOM | 1660 N | ASP | S | 677 | 31.526 | 69.334 | 49.579 | 1.00 | 0.00 |
| ATOM | 1661 CA | ASP | S | 677 | 31.921 | 68.749 | 50.858 | 1.00 | 0.00 |
| ATOM | 1662 C | ASP | S | 677 | 30.840 | 68.725 | 51.907 | 1.00 | 0.00 |
| ATOM | 1663 O | ASP | S | 677 | 30.746 | 67.852 | 52.769 | 1.00 | 0.00 |
| ATOM | 1664 CB | ASP | S | 677 | 33.068 | 69.544 | 51.464 | 1.00 | 0.00 |
| ATOM | 1665 CG | ASP | S | 677 | 34.116 | 68.643 | 52.058 | 1.00 | 0.00 |
| ATOM | 1666 OD1 | ASP | S | 677 | 35.212 | 68.650 | 51.521 | 1.00 | 0.00 |
| ATOM | 1667 OD2 | ASP | S | 677 | 33.860 | 67.947 | 53.041 | 1.00 | 0.00 |
| ATOM | 1668 H | ASP | S | 677 | 31.752 | 70.284 | 49.360 | 1.00 | 0.00 |
| ATOM | 1669 N | LYS | S | 678 | 30.108 | 69.838 | 51.877 | 1.00 | 0.00 |
| ATOM | 1670 CA | LYS | S | 678 | 29.251 | 70.124 | 53.012 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1671 C | LYS | S | 678 | 27.844 | 70.388 | 52.543 | 1.00 | 0.00 |
| ATOM | 1672 O | LYS | S | 678 | 26.934 | 69.613 | 52.807 | 1.00 | 0.00 |
| ATOM | 1673 CB | LYS | S | 678 | 29.809 | 71.301 | 53.829 | 1.00 | 0.00 |
| ATOM | 1674 CG | LYS | S | 678 | 31.244 | 71.151 | 54.369 | 1.00 | 0.00 |
| ATOM | 1675 CD | LYS | S | 678 | 31.418 | 70.389 | 55.694 | 1.00 | 0.00 |
| ATOM | 1676 CE | LYS | S | 678 | 31.087 | 68.892 | 55.702 | 1.00 | 0.00 |
| ATOM | 1677 NZ | LYS | S | 678 | 32.064 | 68.105 | 54.943 | 1.00 | 0.00 |
| ATOM | 1678 H | LYS | S | 678 | 30.115 | 70.431 | 51.068 | 1.00 | 0.00 |
| ATOM | 1679 1HZ | LYS | S | 678 | 32.735 | 68.640 | 54.354 | 1.00 | 0.00 |
| ATOM | 1680 2HZ | LYS | S | 678 | 32.590 | 67.451 | 55.552 | 1.00 | 0.00 |
| ATOM | 1681 3HZ | LYS | S | 678 | 31.522 | 67.507 | 54.282 | 1.00 | 0.00 |
| ATOM | 1682 N | PHE | S | 6781 | 27.701 | 71.504 | 51.820 | 1.00 | 0.00 |
| ATOM | 1683 CA | PHE | S | 6781 | 26.356 | 71.905 | 51.411 | 1.00 | 0.00 |
| ATOM | 1684 C | PHE | S | 6781 | 25.957 | 71.328 | 50.062 | 1.00 | 0.00 |
| ATOM | 1685 O | PHE | S | 6781 | 25.799 | 72.024 | 49.069 | 1.00 | 0.00 |
| ATOM | 1686 CB | PHE | S | 6781 | 26.237 | 73.436 | 51.459 | 1.00 | 0.00 |
| ATOM | 1687 CG | PHE | S | 6781 | 24.792 | 73.876 | 51.352 | 1.00 | 0.00 |
| ATOM | 1688 CD1 | PHE | S | 6781 | 23.882 | 73.553 | 52.382 | 1.00 | 0.00 |
| ATOM | 1689 CD2 | PHE | S | 6781 | 24.379 | 74.606 | 50.216 | 1.00 | 0.00 |
| ATOM | 1690 CE1 | PHE | S | 6781 | 22.537 | 73.957 | 52.272 | 1.00 | 0.00 |
| ATOM | 1691 CE2 | PHE | S | 6781 | 23.035 | 75.011 | 50.103 | 1.00 | 0.00 |
| ATOM | 1692 CZ | PHE | S | 6781 | 22.127 | 74.680 | 51.131 | 1.00 | 0.00 |
| ATOM | 1693 H | PHE | S | 6781 | 28.506 | 71.915 | 51.392 | 1.00 | 0.00 |
| ATOM | 1694 N | ILE | S | 680 | 25.857 | 70.000 | 50.108 | 1.00 | 0.00 |
| ATOM | 1695 CA | ILE | S | 680 | 25.302 | 69.294 | 48.964 | 1.00 | 0.00 |
| ATOM | 1696 C | ILE | S | 680 | 24.912 | 67.930 | 49.484 | 1.00 | 0.00 |
| ATOM | 1697 O | ILE | S | 680 | 25.451 | 67.488 | 50.508 | 1.00 | 0.00 |
| ATOM | 1698 CB | ILE | S | 680 | 26.322 | 69.234 | 47.803 | 1.00 | 0.00 |
| ATOM | 1699 CG1 | ILE | S | 680 | 25.665 | 69.211 | 46.422 | 1.00 | 0.00 |
| ATOM | 1700 CG2 | ILE | S | 680 | 27.318 | 68.076 | 47.960 | 1.00 | 0.00 |
| ATOM | 1701 CD1 | ILE | S | 680 | 26.663 | 69.463 | 45.290 | 1.00 | 0.00 |
| ATOM | 1702 H | ILE | S | 680 | 26.025 | 69.482 | 50.947 | 1.00 | 0.00 |
| ATOM | 1703 N | TYR | S | 681 | 23.998 | 67.308 | 48.764 | 1.00 | 0.00 |
| ATOM | 1704 CA | TYR | S | 681 | 23.676 | 65.918 | 49.043 | 1.00 | 0.00 |
| ATOM | 1705 C | TYR | S | 681 | 23.942 | 65.079 | 47.798 | 1.00 | 0.00 |
| ATOM | 1706 O | TYR | S | 681 | 23.306 | 64.082 | 47.464 | 1.00 | 0.00 |
| ATOM | 1707 CB | TYR | S | 681 | 22.233 | 65.858 | 49.566 | 1.00 | 0.00 |
| ATOM | 1708 CG | TYR | S | 681 | 22.150 | 66.509 | 50.924 | 1.00 | 0.00 |
| ATOM | 1709 CD1 | TYR | S | 681 | 22.274 | 65.697 | 52.068 | 1.00 | 0.00 |
| ATOM | 1710 CD2 | TYR | S | 681 | 21.978 | 67.907 | 51.025 | 1.00 | 0.00 |
| ATOM | 1711 CE1 | TYR | S | 681 | 22.287 | 66.299 | 53.338 | 1.00 | 0.00 |
| ATOM | 1712 CE2 | TYR | S | 681 | 22.007 | 68.512 | 52.293 | 1.00 | 0.00 |
| ATOM | 1713 CZ | TYR | S | 681 | 22.175 | 67.700 | 53.433 | 1.00 | 0.00 |
| ATOM | 1714 OH | TYR | S | 681 | 22.229 | 68.292 | 54.687 | 1.00 | 0.00 |
| ATOM | 1715 H | TYR | S | 681 | 23.518 | 67.809 | 48.046 | 1.00 | 0.00 |
| ATOM | 1716 H | TYR | S | 681 | 22.766 | 69.081 | 54.612 | 1.00 | 0.00 |
| ATOM | 1717 N | ALA | S | 682 | 24.956 | 65.574 | 47.052 | 1.00 | 0.00 |
| ATOM | 1718 CA | ALA | S | 682 | 25.259 | 65.127 | 45.686 | 1.00 | 0.00 |
| ATOM | 1719 C | ALA | S | 682 | 25.008 | 63.666 | 45.384 | 1.00 | 0.00 |
| ATOM | 1720 O | ALA | S | 682 | 25.581 | 62.798 | 46.029 | 1.00 | 0.00 |
| ATOM | 1721 CB | ALA | S | 682 | 26.715 | 65.428 | 45.332 | 1.00 | 0.00 |
| ATOM | 1722 H | ALA | S | 682 | 25.348 | 66.407 | 47.435 | 1.00 | 0.00 |
| ATOM | 1723 N | THR | S | 683 | 24.133 | 63.392 | 44.418 | 1.00 | 0.00 |
| ATOM | 1724 CA | THR | S | 683 | 23.975 | 61.977 | 44.113 | 1.00 | 0.00 |
| ATOM | 1725 C | THR | S | 683 | 25.121 | 61.425 | 43.255 | 1.00 | 0.00 |
| ATOM | 1726 O | THR | S | 683 | 26.125 | 62.104 | 43.032 | 1.00 | 0.00 |
| ATOM | 1727 CB | THR | S | 683 | 22.531 | 31.705 | 43.610 | 1.00 | 0.00 |
| ATOM | 1728 OG1 | THR | S | 683 | 22.178 | 60.316 | 43.674 | 1.00 | 0.00 |
| ATOM | 1729 CG2 | THR | S | 683 | 22.203 | 62.246 | 42.226 | 1.00 | 0.00 |
| ATOM | 1730 H | THR | S | 683 | 23.820 | 64.093 | 43.771 | 1.00 | 0.00 |
| ATOM | 1731 HG1 | THR | S | 683 | 22.584 | 59.960 | 44.466 | 1.00 | 0.00 |
| ATOM | 1732 N | VAL | S | 684 | 24.944 | 60.160 | 42.839 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1733 CA | VAL | S | 684 | 25.659 | 59.574 | 41.707 | 1.00 | 0.00 |
| ATOM | 1734 C | VAL | S | 684 | 24.991 | 58.294 | 41.319 | 1.00 | 0.00 |
| ATOM | 1735 O | VAL | S | 684 | 24.318 | 57.610 | 42.087 | 1.00 | 0.00 |
| ATOM | 1736 CB | VAL | S | 684 | 27.138 | 59.197 | 41.882 | 1.00 | 0.00 |
| ATOM | 1737 CG1 | VAL | S | 684 | 28.068 | 60.270 | 41.342 | 1.00 | 0.00 |
| ATOM | 1738 CG2 | VAL | S | 684 | 27.468 | 58.615 | 43.251 | 1.00 | 0.00 |
| ATOM | 1739 H | VAL | S | 684 | 24.105 | 59.684 | 43.116 | 1.00 | 0.00 |
| ATOM | 1740 N | LYS | S | 685 | 25.263 | 57.970 | 40.057 | 1.00 | 0.00 |
| ATOM | 1741 CA | LYS | S | 685 | 24.690 | 56.709 | 39.623 | 1.00 | 0.00 |
| ATOM | 1742 C | LYS | S | 685 | 25.620 | 55.591 | 40.020 | 1.00 | 0.00 |
| ATOM | 1743 O | LYS | S | 685 | 26.799 | 55.815 | 40.326 | 1.00 | 0.00 |
| ATOM | 1744 CB | LYS | S | 685 | 24.315 | 56.761 | 38.140 | 1.00 | 0.00 |
| ATOM | 1745 CG | LYS | S | 685 | 23.013 | 57.545 | 37.886 | 1.00 | 0.00 |
| ATOM | 1746 CD | LYS | S | 685 | 23.025 | 59.010 | 38.343 | 1.00 | 0.00 |
| ATOM | 1747 CE | LYS | S | 685 | 21.693 | 59.734 | 38.258 | 1.00 | 0.00 |
| ATOM | 1748 NZ | LYS | S | 685 | 21.385 | 59.972 | 36.856 | 1.00 | 0.00 |
| ATOM | 1749 H | LYS | S | 685 | 25.831 | 58.580 | 39.497 | 1.00 | 0.00 |
| ATOM | 1750 1HZ | LYS | S | 685 | 20.526 | 59.526 | 36.500 | 1.00 | 0.00 |
| ATOM | 1751 2HZ | LYS | S | 685 | 21.353 | 60.989 | 36.633 | 1.00 | 0.00 |
| ATOM | 1752 3HZ | LYS | S | 685 | 22.167 | 59.645 | 36.259 | 1.00 | 0.00 |
| ATOM | 1753 N | GLN | S | 686 | 25.001 | 54.413 | 40.089 | 1.00 | 0.00 |
| ATOM | 1754 CA | GLN | S | 686 | 25.666 | 53.337 | 40.793 | 1.00 | 0.00 |
| ATOM | 1755 C | GLN | S | 686 | 26.936 | 52.902 | 40.112 | 1.00 | 0.00 |
| ATOM | 1756 O | GLN | S | 686 | 27.153 | 53.060 | 38.912 | 1.00 | 0.00 |
| ATOM | 1757 CB | GLN | S | 686 | 24.676 | 52.198 | 41.086 | 1.00 | 0.00 |
| ATOM | 1758 CG | GLN | S | 686 | 24.984 | 51.268 | 42.276 | 1.00 | 0.00 |
| ATOM | 1759 CD | GLN | S | 686 | 25.397 | 52.052 | 43.515 | 1.00 | 0.00 |
| ATOM | 1760 OE1 | GLN | S | 686 | 26.512 | 52.538 | 43.610 | 1.00 | 0.00 |
| ATOM | 1761 NE2 | GLN | S | 686 | 24.500 | 52.121 | 44.499 | 1.00 | 0.00 |
| ATOM | 1762 H | GLN | S | 686 | 24.089 | 54.305 | 39.703 | 1.00 | 0.00 |
| ATOM | 1763 1HE2 | GLN | S | 686 | 24.655 | 52.726 | 45.284 | 1.00 | 0.00 |
| ATOM | 1764 2HE2 | GLN | S | 686 | 23.652 | 51.596 | 44.462 | 1.00 | 0.00 |
| ATOM | 1765 N | SER | S | 687 | 27.827 | 52.411 | 40.988 | 1.00 | 0.00 |
| ATOM | 1766 CA | SER | S | 687 | 29.128 | 51.889 | 40.576 | 1.00 | 0.00 |
| ATOM | 1767 C | SER | S | 687 | 29.931 | 52.713 | 39.576 | 1.00 | 0.00 |
| ATOM | 1768 O | SER | S | 687 | 30.706 | 52.246 | 38.744 | 1.00 | 0.00 |
| ATOM | 1769 CB | SER | S | 687 | 28.995 | 50.423 | 40.183 | 1.00 | 0.00 |
| ATOM | 1770 OG | SER | S | 687 | 30.179 | 49.745 | 40.615 | 1.00 | 0.00 |
| ATOM | 1771 H | SER | S | 687 | 27.555 | 52.341 | 41.949 | 1.00 | 0.00 |
| ATOM | 1772 HG | SER | S | 687 | 30.047 | 48.835 | 40.360 | 1.00 | 0.00 |
| ATOM | 1773 N | SER | S | 688 | 29.746 | 54.017 | 39.729 | 1.00 | 0.00 |
| ATOM | 1774 CA | SER | S | 688 | 30.401 | 54.940 | 38.834 | 1.00 | 0.00 |
| ATOM | 1775 C | SER | S | 688 | 31.868 | 55.132 | 39.185 | 1.00 | 0.00 |
| ATOM | 1776 O | SER | S | 688 | 32.298 | 55.008 | 40.340 | 1.00 | 0.00 |
| ATOM | 1777 CB | SER | S | 688 | 29.585 | 56.240 | 38.861 | 1.00 | 0.00 |
| ATOM | 1778 OG | SER | S | 688 | 29.995 | 57.118 | 37.806 | 1.00 | 0.00 |
| ATOM | 1779 H | SER | S | 688 | 29.133 | 54.349 | 40.441 | 1.00 | 0.00 |
| ATOM | 1780 HG | SER | S | 688 | 29.780 | 56.645 | 36.995 | 1.00 | 0.00 |
| ATOM | 1781 N | VAL | S | 689 | 32.597 | 55.472 | 38.110 | 1.00 | 0.00 |
| ATOM | 1782 CA | VAL | S | 689 | 33.337 | 56.742 | 38.000 | 1.00 | 0.00 |
| ATOM | 1783 C | VAL | S | 689 | 33.414 | 57.580 | 39.278 | 1.00 | 0.00 |
| ATOM | 1784 O | VAL | S | 689 | 34.406 | 57.635 | 40.005 | 1.00 | 0.00 |
| ATOM | 1785 CB | VAL | S | 689 | 32.712 | 57.580 | 36.853 | 1.00 | 0.00 |
| ATOM | 1786 CG1 | VAL | S | 689 | 33.442 | 58.887 | 36.576 | 1.00 | 0.00 |
| ATOM | 1787 CG2 | VAL | S | 689 | 32.445 | 56.779 | 35.578 | 1.00 | 0.00 |
| ATOM | 1788 H | VAL | S | 689 | 32.437 | 54.935 | 37.287 | 1.00 | 0.00 |
| ATOM | 1789 N | ASP | S | 690 | 32.281 | 58.260 | 39.539 | 1.00 | 0.00 |
| ATOM | 1790 CA | ASP | S | 690 | 32.296 | 59.125 | 40.718 | 1.00 | 0.00 |
| ATOM | 1791 C | ASP | S | 690 | 31.748 | 58.481 | 41.985 | 1.00 | 0.00 |
| ATOM | 1792 O | ASP | S | 690 | 31.366 | 59.107 | 42.968 | 1.00 | 0.00 |
| ATOM | 1793 CB | ASP | S | 690 | 31.678 | 60.500 | 40.404 | 1.00 | 0.00 |
| ATOM | 1794 CG | ASP | S | 690 | 31.915 | 61.497 | 41.535 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1795 OD1 | ASP | S | 690 | 31.116 | 62.418 | 41.686 | 1.00 | 0.00 |
| ATOM | 1796 OD2 | ASP | S | 690 | 32.871 | 61.333 | 42.294 | 1.00 | 0.00 |
| ATOM | 1797 H | ASP | S | 690 | 31.500 | 58.264 | 38.915 | 1.00 | 0.00 |
| ATOM | 1798 N | ILE | S | 691 | 31.773 | 57.154 | 41.976 | 1.00 | 0.00 |
| ATOM | 1799 CA | ILE | S | 691 | 32.015 | 56.569 | 43.287 | 1.00 | 0.00 |
| ATOM | 1800 C | ILE | S | 691 | 33.498 | 56.550 | 43.569 | 1.00 | 0.00 |
| ATOM | 1801 O | ILE | S | 691 | 33.942 | 56.904 | 44.651 | 1.00 | 0.00 |
| ATOM | 1802 CB | ILE | S | 691 | 31.407 | 55.172 | 43.419 | 1.00 | 0.00 |
| ATOM | 1803 CG1 | ILE | S | 691 | 29.904 | 55.300 | 43.197 | 1.00 | 0.00 |
| ATOM | 1804 CG2 | ILE | S | 691 | 31.707 | 54.579 | 44.806 | 1.00 | 0.00 |
| ATOM | 1805 CD1 | ILE | S | 691 | 29.181 | 54.009 | 43.548 | 1.00 | 0.00 |
| ATOM | 1806 H | ILE | S | 691 | 31.887 | 56.675 | 41.117 | 1.00 | 0.00 |
| ATOM | 1807 N | TYR | S | 692 | 34.257 | 56.116 | 42.540 | 1.00 | 0.00 |
| ATOM | 1808 CA | TYR | S | 692 | 35.715 | 56.051 | 42.692 | 1.00 | 0.00 |
| ATOM | 1809 C | TYR | S | 692 | 36.354 | 57.362 | 43.107 | 1.00 | 0.00 |
| ATOM | 1810 O | TYR | S | 692 | 36.975 | 57.463 | 44.163 | 1.00 | 0.00 |
| ATOM | 1811 CB | TYR | S | 692 | 36.404 | 55.537 | 41.420 | 1.00 | 0.00 |
| ATOM | 1812 CG | TYR | S | 692 | 36.034 | 54.104 | 41.120 | 1.00 | 0.00 |
| ATOM | 1813 CD1 | TYR | S | 692 | 36.525 | 53.079 | 41.955 | 1.00 | 0.00 |
| ATOM | 1814 CD2 | TYR | S | 692 | 35.220 | 53.830 | 40.003 | 1.00 | 0.00 |
| ATOM | 1815 CE1 | TYR | S | 692 | 36.196 | 51.746 | 41.663 | 1.00 | 0.00 |
| ATOM | 1816 CE2 | TYR | S | 692 | 34.889 | 52.496 | 39.712 | 1.00 | 0.00 |
| ATOM | 1817 CZ | TYR | S | 692 | 35.382 | 51.471 | 40.547 | 1.00 | 0.00 |
| ATOM | 1818 OH | TYR | S | 692 | 35.059 | 50.159 | 40.273 | 1.00 | 0.00 |
| ATOM | 1819 H | TYR | S | 692 | 33.836 | 55.925 | 41.656 | 1.00 | 0.00 |
| ATOM | 1820 HH | TYR | S | 692 | 34.392 | 50.198 | 39.588 | 1.00 | 0.00 |
| ATOM | 1821 N | PHE | S | 693 | 36.153 | 58.380 | 42.245 | 1.00 | 0.00 |
| ATOM | 1822 CA | PHE | S | 693 | 36.638 | 59.734 | 42.532 | 1.00 | 0.00 |
| ATOM | 1823 C | PHE | S | 693 | 36.291 | 60.206 | 43.935 | 1.00 | 0.00 |
| ATOM | 1824 O | PHE | S | 693 | 37.138 | 60.525 | 44.770 | 1.00 | 0.00 |
| ATOM | 1825 CB | PHE | S | 693 | 36.084 | 60.684 | 41.459 | 1.00 | 0.00 |
| ATOM | 1826 CG | PHE | S | 693 | 36.698 | 62.065 | 41.520 | 1.00 | 0.00 |
| ATOM | 1827 CD1 | PHE | S | 693 | 37.907 | 62.318 | 40.835 | 1.00 | 0.00 |
| ATOM | 1828 CD2 | PHE | S | 693 | 36.041 | 63.086 | 42.241 | 1.00 | 0.00 |
| ATOM | 1829 CE1 | PHE | S | 693 | 38.458 | 63.613 | 40.854 | 1.00 | 0.00 |
| ATOM | 1830 CE2 | PHE | S | 693 | 36.592 | 64.382 | 42.262 | 1.00 | 0.00 |
| ATOM | 1831 CZ | PHE | S | 693 | 37.790 | 64.624 | 41.562 | 1.00 | 0.00 |
| ATOM | 1832 H | PHE | S | 693 | 35.559 | 58.210 | 41.458 | 1.00 | 0.00 |
| ATOM | 1833 N | ARG | S | 694 | 34.962 | 60.211 | 44.166 | 1.00 | 0.00 |
| ATOM | 1834 CA | ARG | S | 694 | 34.403 | 60.480 | 45.495 | 1.00 | 0.00 |
| ATOM | 1835 C | ARG | S | 694 | 34.994 | 59.664 | 46.631 | 1.00 | 0.00 |
| ATOM | 1836 O | ARG | S | 694 | 35.185 | 60.150 | 47.736 | 1.00 | 0.00 |
| ATOM | 1837 CB | ARG | S | 694 | 32.883 | 60.294 | 45.503 | 1.00 | 0.00 |
| ATOM | 1838 CG | ARG | S | 694 | 32.101 | 61.030 | 46.602 | 1.00 | 0.00 |
| ATOM | 1839 CD | ARG | S | 694 | 31.938 | 62.526 | 46.315 | 1.00 | 0.00 |
| ATOM | 1840 NE | ARG | S | 694 | 31.013 | 63.203 | 47.228 | 1.00 | 0.00 |
| ATOM | 1841 CZ | ARG | S | 694 | 30.586 | 64.452 | 46.934 | 1.00 | 0.00 |
| ATOM | 1842 NH1 | ARG | S | 694 | 29.613 | 65.009 | 47.658 | 1.00 | 0.00 |
| ATOM | 1843 NH2 | ARG | S | 694 | 31.133 | 65.137 | 45.937 | 1.00 | 0.00 |
| ATOM | 1844 H | ARG | S | 694 | 34.357 | 60.153 | 43.365 | 1.00 | 0.00 |
| ATOM | 1845 HE | ARG | S | 694 | 30.724 | 62.743 | 48.070 | 1.00 | 0.00 |
| ATOM | 1846 1HH1 | ARG | S | 694 | 29.352 | 65.965 | 47.495 | 1.00 | 0.00 |
| ATOM | 1847 2HH1 | ARG | S | 694 | 29.133 | 64.521 | 48.390 | 1.00 | 0.00 |
| ATOM | 1848 1HH2 | ARG | S | 694 | 30.768 | 66.018 | 45.652 | 1.00 | 0.00 |
| ATOM | 1849 2HH2 | ARG | S | 694 | 31.958 | 64.797 | 45.347 | 1.00 | 0.00 |
| ATOM | 1850 N | ARG | S | 695 | 35.297 | 58.394 | 46.332 | 1.00 | 0.00 |
| ATOM | 1851 CA | ARG | S | 695 | 35.772 | 57.522 | 47.394 | 1.00 | 0.00 |
| ATOM | 1852 C | ARG | S | 695 | 37.022 | 58.050 | 48.052 | 1.00 | 0.00 |
| ATOM | 1853 O | ARG | S | 695 | 37.086 | 58.112 | 49.268 | 1.00 | 0.00 |
| ATOM | 1854 CB | ARG | S | 695 | 35.976 | 56.088 | 46.901 | 1.00 | 0.00 |
| ATOM | 1855 CG | ARG | S | 695 | 36.034 | 55.074 | 48.042 | 1.00 | 0.00 |
| ATOM | 1856 CD | ARG | S | 695 | 34.733 | 54.303 | 48.300 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1857 NE | ARG | S | 695 | 33.532 | 55.124 | 48.519 | 1.00 | 0.00 |
| ATOM | 1858 CZ | ARG | S | 695 | 33.248 | 55.723 | 49.705 | 1.00 | 0.00 |
| ATOM | 1859 NH1 | ARG | S | 695 | 32.005 | 56.132 | 49.932 | 1.00 | 0.00 |
| ATOM | 1860 NH2 | ARG | S | 695 | 34.177 | 55.903 | 50.633 | 1.00 | 0.00 |
| ATOM | 1861 H | ARG | S | 695 | 35.230 | 58.064 | 45.392 | 1.00 | 0.00 |
| ATOM | 1862 HE | ARG | S | 695 | 32.848 | 55.078 | 47.787 | 1.00 | 0.00 |
| ATOM | 1863 1HH1 | ARG | S | 695 | 31.716 | 56.522 | 50.807 | 1.00 | 0.00 |
| ATOM | 1864 2HH1 | ARG | S | 695 | 31.311 | 56.061 | 49.212 | 1.00 | 0.00 |
| ATOM | 1865 1HH2 | ARG | S | 695 | 33.954 | 56.195 | 51.561 | 1.00 | 0.00 |
| ATOM | 1866 2HH2 | ARG | S | 695 | 35.143 | 55.762 | 50.417 | 1.00 | 0.00 |
| ATOM | 1867 N | GLN | S | 696 | 37.966 | 58.474 | 47.190 | 1.00 | 0.00 |
| ATOM | 1868 CA | GLN | S | 696 | 39.249 | 58.940 | 47.717 | 1.00 | 0.00 |
| ATOM | 1869 C | GLN | S | 696 | 39.354 | 60.451 | 47.704 | 1.00 | 0.00 |
| ATOM | 1870 O | GLN | S | 696 | 39.429 | 61.147 | 48.708 | 1.00 | 0.00 |
| ATOM | 1871 CB | GLN | S | 696 | 40.405 | 58.344 | 46.900 | 1.00 | 0.00 |
| ATOM | 1872 CG | GLN | S | 696 | 40.179 | 56.932 | 46.346 | 1.00 | 0.00 |
| ATOM | 1873 CD | GLN | S | 696 | 40.076 | 55.924 | 47.470 | 1.00 | 0.00 |
| ATOM | . OE1 | GLN | S | 696 | 39.191 | 55.959 | 48.314 | 1.00 | 0.00 |
| ATOM | 1875 NE2 | GLN | S | 696 | 41.041 | 55.007 | 47.440 | 1.00 | 0.00 |
| ATOM | 1876 H | GLN | S | 696 | 37.720 | 58.479 | 46.219 | 1.00 | 0.00 |
| ATOM | 1877 1HE2 | GLN | S | 696 | 41.068 | 54.313 | 48.158 | 1.00 | 0.00 |
| ATOM | 1878 2HE2 | GLN | S | 696 | 41.724 | 55.036 | 46.713 | 1.00 | 0.00 |
| ATOM | 1879 N | VAL | S | 697 | 39.331 | 60.940 | 46.459 | 1.00 | 0.00 |
| ATOM | 1880 CA | VAL | S | 697 | 39.584 | 62.359 | 46.212 | 1.00 | 0.00 |
| ATOM | 1881 C | VAL | S | 697 | 38.477 | 63.251 | 46.754 | 1.00 | 0.00 |
| ATOM | 1882 O | VAL | S | 697 | 38.657 | 64.411 | 47.113 | 1.00 | 0.00 |
| ATOM | 1883 CB | VAL | S | 697 | 39.792 | 62.597 | 44.704 | 1.00 | 0.00 |
| ATOM | 1884 CG1 | VAL | S | 697 | 40.276 | 64.018 | 44.399 | 1.00 | 0.00 |
| ATOM | 1885 CG2 | VAL | S | 697 | 40.736 | 61.555 | 44.096 | 1.00 | 0.00 |
| ATOM | 1886 H | VAL | S | 697 | 38.966 | 60.359 | 45.733 | 1.00 | 0.00 |
| ATOM | 1887 N | GLU | S | 698 | 37.283 | 62.962 | 46.803 | 1.00 | 0.00 |
| ATOM | 1888 CA | GLU | S | 698 | 36.286 | 63.423 | 47.535 | 1.00 | 0.00 |
| ATOM | 1889 C | GLU | S | 698 | 35.847 | 62.738 | 48.813 | 1.00 | 0.00 |
| ATOM | 1890 O | GLU | S | 698 | 34.708 | 62.841 | 49.262 | 1.00 | 0.00 |
| ATOM | 1891 CB | GLU | S | 698 | 35.110 | 63.831 | 46.650 | 1.00 | 0.00 |
| ATOM | 1892 CG | GLU | S | 698 | 35.363 | 64.995 | 45.684 | 1.00 | 0.00 |
| ATOM | 1893 CD | GLU | S | 698 | 34.051 | 65.397 | 45.027 | 1.00 | 0.00 |
| ATOM | 1894 OE1 | GLU | S | 698 | 33.498 | 64.626 | 44.257 | 1.00 | 0.00 |
| ATOM | 1895 OE2 | GLU | S | 698 | 33.543 | 66.483 | 45.278 | 1.00 | 0.00 |
| ATOM | 1896 H | GLU | S | 698 | 37.168 | 61.714 | 46.500 | 1.00 | 0.00 |
| ATOM | 1897 N | LEU | S | 699 | 36.832 | 62.076 | 49.433 | 1.00 | 0.00 |
| ATOM | 1898 CA | LEU | S | 699 | 36.621 | 61.648 | 50.810 | 1.00 | 0.00 |
| ATOM | 1899 C | LEU | S | 699 | 37.059 | 62.712 | 51.782 | 1.00 | 0.00 |
| ATOM | 1900 O | LEU | S | 699 | 37.845 | 62.520 | 52.700 | 1.00 | 0.00 |
| ATOM | 1901 CB | LEU | S | 699 | 37.329 | 60.342 | 51.149 | 1.00 | 0.00 |
| ATOM | 1902 CG | LEU | S | 699 | 36.673 | 59.583 | 52.308 | 1.00 | 0.00 |
| ATOM | 1903 CD1 | LEU | S | 699 | 35.205 | 59.256 | 52.023 | 1.00 | 0.00 |
| ATOM | 1904 CD2 | LEU | S | 699 | 37.473 | 58.336 | 52.690 | 1.00 | 0.00 |
| ATOM | 1905 H | LEU | S | 699 | 37.739 | 62.018 | 49.023 | 1.00 | 0.00 |
| ATOM | 1906 N | SER | S | 700 | 36.487 | 63.884 | 51.546 | 1.00 | 0.00 |
| ATOM | 1907 CA | SER | S | 700 | 36.329 | 64.638 | 52.769 | 1.00 | 0.00 |
| ATOM | 1908 C | SER | S | 700 | 34.941 | 64.286 | 53.276 | 1.00 | 0.00 |
| ATOM | 1909 O | SER | S | 700 | 34.280 | 63.441 | 52.673 | 1.00 | 0.00 |
| ATOM | 1910 CB | SER | S | 700 | 36.583 | 66.102 | 52.456 | 1.00 | 0.00 |
| ATOM | 1911 OG | SER | S | 700 | 37.677 | 66.218 | 51.520 | 1.00 | 0.00 |
| ATOM | 1912 H | SER | S | 700 | 35.848 | 63.982 | 50.787 | 1.00 | 0.00 |
| ATOM | 1913 HG | SER | S | 700 | 38.317 | 65.572 | 51.825 | 1.00 | 0.00 |
| ATOM | 1914 N | THR | S | 701 | 34.527 | 64.913 | 54.379 | 1.00 | 0.00 |
| ATOM | 1915 CA | THR | S | 701 | 33.290 | 64.467 | 55.017 | 1.00 | 0.00 |
| ATOM | 1916 C | THR | S | 701 | 32.005 | 64.803 | 54.264 | 1.00 | 0.00 |
| ATOM | 1917 O | THR | S | 701 | 31.299 | 65.724 | 54.658 | 1.00 | 0.00 |
| ATOM | 1918 CB | THR | S | 701 | 33.296 | 65.092 | 56.411 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1919 OG1 | THR | S | 701 | 33.757 | 66.457 | 56.324 | 1.00 | 0.00 |
| ATOM | 1920 CG2 | THR | S | 701 | 34.196 | 64.301 | 57.363 | 1.00 | 0.00 |
| ATOM | 1921 H | THR | S | 701 | 35.034 | 65.669 | 54.794 | 1.00 | 0.00 |
| ATOM | 1922 HG1 | THR | S | 701 | 34.101 | 66.689 | 57.189 | 1.00 | 0.00 |
| ATOM | 1923 N | MET | S | 702 | 31.735 | 64.073 | 53.185 | 1.00 | 0.00 |
| ATOM | 1924 CA | MET | S | 702 | 30.680 | 64.555 | 52.304 | 1.00 | 0.00 |
| ATOM | 1925 C | MET | S | 702 | 29.384 | 63.784 | 52.387 | 1.00 | 0.00 |
| ATOM | 1926 O | MET | S | 702 | 29.349 | 62.559 | 52.311 | 1.00 | 0.00 |
| ATOM | 1927 CB | MET | S | 702 | 31.158 | 64.565 | 50.849 | 1.00 | 0.00 |
| ATOM | 1928 CG | MET | S | 702 | 32.470 | 65.316 | 50.629 | 1.00 | 0.00 |
| ATOM | 1929 SD | MET | S | 702 | 32.899 | 65.481 | 48.892 | 1.00 | 0.00 |
| ATOM | 1930 CE | MET | S | 702 | 34.345 | 66.530 | 49.083 | 1.00 | 0.00 |
| ATOM | 1931 H | MET | S | 702 | 32.316 | 63.300 | 52.938 | 1.00 | 0.00 |
| ATOM | 1932 N | TYR | S | 703 | 28.302 | 64.571 | 52.463 | 1.00 | 0.00 |
| ATOM | 1933 CA | TYR | S | 703 | 27.061 | 63.922 | 52.062 | 1.00 | 0.00 |
| ATOM | 1934 C | TYR | S | 703 | 27.080 | 63.793 | 50.554 | 1.00 | 0.00 |
| ATOM | 1935 O | TYR | S | 703 | 27.656 | 64.621 | 49.840 | 1.00 | 0.00 |
| ATOM | 1936 CB | TYR | S | 703 | 25.821 | 64.657 | 52.587 | 1.00 | 0.00 |
| ATOM | 1937 CG | TYR | S | 703 | 24.861 | 63.672 | 53.233 | 1.00 | 0.00 |
| ATOM | 1938 CD1 | TYR | S | 703 | 24.539 | 63.828 | 54.597 | 1.00 | 0.00 |
| ATOM | 1939 CD2 | TYR | S | 703 | 24.310 | 62.624 | 52.466 | 1.00 | 0.00 |
| ATOM | 1940 CE1 | TYR | S | 703 | 23.660 | 62.913 | 55.208 | 1.00 | 0.00 |
| ATOM | 1941 CE2 | TYR | S | 703 | 23.443 | 61.702 | 53.076 | 1.00 | 0.00 |
| ATOM | 1942 CZ | TYR | S | 703 | 23.132 | 61.851 | 54.442 | 1.00 | 0.00 |
| ATOM | 1943 OH | TYR | S | 703 | 22.302 | 60.916 | 55.038 | 1.00 | 0.00 |
| ATOM | 1944 H | TYR | S | 703 | 28.424 | 65.562 | 52.430 | 1.00 | 0.00 |
| ATOM | 1945 HH | TYR | S | 703 | 21.883 | 61.314 | 55.797 | 1.00 | 0.00 |
| ATOM | 1946 N | ARG | S | 704 | 26.545 | 62.675 | 50.124 | 1.00 | 0.00 |
| ATOM | 1947 CA | ARG | S | 704 | 26.666 | 62.236 | 48.748 | 1.00 | 0.00 |
| ATOM | 1948 C | ARG | S | 704 | 25.722 | 61.084 | 48.672 | 1.00 | 0.00 |
| ATOM | 1949 O | ARG | S | 704 | 25.996 | 59.999 | 49.171 | 1.00 | 0.00 |
| ATOM | 1950 CB | ARG | S | 704 | 28.133 | 61.876 | 48.432 | 1.00 | 0.00 |
| ATOM | 1951 CG | ARG | S | 704 | 28.552 | 60.776 | 47.440 | 1.00 | 0.00 |
| ATOM | 1952 CD | ARG | S | 704 | 28.021 | 60.754 | 46.000 | 1.00 | 0.00 |
| ATOM | 1953 NE | ARG | S | 704 | 28.103 | 62.010 | 45.247 | 1.00 | 0.00 |
| ATOM | 1954 CZ | ARG | S | 704 | 28.882 | 62.131 | 44.143 | 1.00 | 0.00 |
| ATOM | 1955 NH1 | ARG | S | 704 | 28.670 | 63.117 | 43.285 | 1.00 | 0.00 |
| ATOM | 1956 NH2 | ARG | S | 704 | 29.838 | 61.272 | 43.877 | 1.00 | 0.00 |
| ATOM | 1957 H | ARG | S | 704 | 26.124 | 62.100 | 50.824 | 1.00 | 0.00 |
| ATOM | 1958 HE | ARG | S | 704 | 27.353 | 62.657 | 45.378 | 1.00 | 0.00 |
| ATOM | 1959 1HH1 | ARG | S | 704 | 29.298 | 63.219 | 42.499 | 1.00 | 0.00 |
| ATOM | 1960 2HH1 | ARG | S | 704 | 27.876 | 63.720 | 43.366 | 1.00 | 0.00 |
| ATOM | 1961 1HH2 | ARG | S | 704 | 30.435 | 61.403 | 43.076 | 1.00 | 0.00 |
| ATOM | 1962 2HH2 | ARG | S | 704 | 29.986 | 60.474 | 44.448 | 1.00 | 0.00 |
| ATOM | 1963 N | HIS | S | 705 | 24.564 | 61.388 | 48.076 | 1.00 | 0.00 |
| ATOM | 1964 CA | HIS | S | 705 | 23.554 | 60.360 | 47.845 | 1.00 | 0.00 |
| ATOM | 1965 C | HIS | S | 705 | 24.052 | 59.379 | 46.799 | 1.00 | 0.00 |
| ATOM | 1966 O | HIS | S | 705 | 23.858 | 59.498 | 45.593 | 1.00 | 0.00 |
| ATOM | 1967 CB | HIS | S | 705 | 22.226 | 61.012 | 47.437 | 1.00 | 0.00 |
| ATOM | 1968 CG | HIS | S | 705 | 21.600 | 61.818 | 48.563 | 1.00 | 0.00 |
| ATOM | 1969 ND1 | HIS | S | 705 | 20.457 | 62.523 | 48.434 | 1.00 | 0.00 |
| ATOM | 1970 CD2 | HIS | S | 705 | 22.050 | 61.961 | 49.880 | 1.00 | 0.00 |
| ATOM | 1971 CE1 | HIS | S | 705 | 20.184 | 63.091 | 49.652 | 1.00 | 0.00 |
| ATOM | 1972 NE2 | HIS | S | 705 | 21.173 | 62.752 | 50.547 | 1.00 | 0.00 |
| ATOM | 1973 H | HIS | S | 705 | 24.404 | 62.322 | 47.742 | 1.00 | 0.00 |
| ATOM | 1974 HD1 | HIS | S | 705 | 19.939 | 62.682 | 47.618 | 1.00 | 0.00 |
| ATOM | 1975 N | MET | S | 706 | 24.815 | 58.422 | 47.321 | 1.00 | 0.00 |
| ATOM | 1976 CA | MET | S | 706 | 25.538 | 57.546 | 46.409 | 1.00 | 0.00 |
| ATOM | 1977 C | MET | S | 706 | 24.614 | 56.488 | 45.862 | 1.00 | 0.00 |
| ATOM | 1978 O | MET | S | 706 | 24.506 | 55.392 | 46.400 | 1.00 | 0.00 |
| ATOM | 1979 CB | MET | S | 706 | 26.721 | 56.930 | 47.150 | 1.00 | 0.00 |
| ATOM | 1980 CG | MET | S | 706 | 27.276 | 56.268 | 46.215 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1981 SD | MET | S | 706 | 29.060 | 55.467 | 47.114 | 1.00 | 0.00 |
| ATOM | 1982 CE | MET | S | 706 | 28.165 | 53.985 | 47.619 | 1.00 | 0.00 |
| ATOM | 1983 H | MET | S | 706 | 24.957 | 58.417 | 48.313 | 1.00 | 0.00 |
| ATOM | 1984 N | GLU | S | 707 | 23.871 | 56.880 | 44.836 | 1.00 | 0.00 |
| ATOM | 1985 CA | GLU | S | 707 | 22.602 | 56.198 | 44.745 | 1.00 | 0.00 |
| ATOM | 1986 C | GLU | S | 707 | 22.613 | 54.891 | 44.001 | 1.00 | 0.00 |
| ATOM | 1987 O | GLU | S | 707 | 23.449 | 54.631 | 43.149 | 1.00 | 0.00 |
| ATOM | 1988 CB | GLU | S | 707 | 21.537 | 57.197 | 44.287 | 1.00 | 0.00 |
| ATOM | 1989 CG | GLU | S | 707 | 20.112 | 56.889 | 44.759 | 1.00 | 0.00 |
| ATOM | 1990 CD | GLU | S | 707 | 20.132 | 56.469 | 46.216 | 1.00 | 0.00 |
| ATOM | 1991 OE1 | GLU | S | 707 | 20.644 | 57.210 | 47.057 | 1.00 | 0.00 |
| ATOM | 1992 OE2 | GLU | S | 707 | 19.658 | 55.373 | 46.493 | 1.00 | 0.00 |
| ATOM | 1993 H | GLU | S | 707 | 24.044 | 57.713 | 44.311 | 1.00 | 0.00 |
| ATOM | 1994 N | LYS | S | 708 | 21.614 | 54.087 | 44.400 | 1.00 | 0.00 |
| ATOM | 1995 CA | LYS | S | 708 | 21.377 | 52.758 | 43.845 | 1.00 | 0.00 |
| ATOM | 1996 C | LYS | S | 708 | 20.952 | 52.796 | 42.387 | 1.00 | 0.00 |
| ATOM | 1997 O | LYS | S | 708 | 21.744 | 53.061 | 41.518 | 1.00 | 0.00 |
| ATOM | 1998 CB | LYS | S | 708 | 20.423 | 51.961 | 44.749 | 1.00 | 0.00 |
| ATOM | 1999 CG | LYS | S | 708 | 20.680 | 52.212 | 46.239 | 1.00 | 0.00 |
| ATOM | 2000 CD | LYS | S | 708 | 19.653 | 51.624 | 47.213 | 1.00 | 0.00 |
| ATOM | 2001 CE | LYS | S | 708 | 18.169 | 51.861 | 46.885 | 1.00 | 0.00 |
| ATOM | 2002 NZ | LYS | S | 708 | 17.884 | 53.226 | 46.423 | 1.00 | 0.00 |
| ATOM | 2003 H | LYS | S | 708 | 21.011 | 54.452 | 45.111 | 1.00 | 0.00 |
| ATOM | 2004 1HZ | LYS | S | 708 | 18.480 | 53.967 | 46.841 | 1.00 | 0.00 |
| ATOM | 2005 2HZ | LYS | S | 708 | 17.983 | 53.256 | 45.389 | 1.00 | 0.00 |
| ATOM | 2006 3HZ | LYS | S | 708 | 16.873 | 53.459 | 46.518 | 1.00 | 0.00 |
| ATOM | 2007 N | HIS | S | 709 | 19.679 | 52.534 | 42.110 | 1.00 | 0.00 |
| ATOM | 2008 CA | HIS | S | 709 | 19.385 | 52.517 | 40.691 | 1.00 | 0.00 |
| ATOM | 2009 C | HIS | S | 709 | 19.359 | 53.912 | 40.092 | 1.00 | 0.00 |
| ATOM | 2010 O | HIS | S | 709 | 18.790 | 54.964 | 40.629 | 1.00 | 0.00 |
| ATOM | 2011 CB | HIS | S | 709 | 18.105 | 51.713 | 40.439 | 1.00 | 0.00 |
| ATOM | 2012 CG | HIS | S | 709 | 17.851 | 51.537 | 38.961 | 1.00 | 0.00 |
| ATOM | 2013 ND1 | HIS | S | 709 | 16.804 | 52.101 | 38.342 | 1.00 | 0.00 |
| ATOM | 2014 CD2 | HIS | S | 709 | 18.591 | 50.808 | 38.023 | 1.00 | 0.00 |
| ATOM | 2015 CE1 | HIS | S | 709 | 16.865 | 51.744 | 37.023 | 1.00 | 0.00 |
| ATOM | 2016 NE2 | HIS | S | 709 | 17.963 | 50.947 | 36.827 | 1.00 | 0.00 |
| ATOM | 2017 H | HIS | S | 709 | 18.960 | 52.645 | 42.793 | 1.00 | 0.00 |
| ATOM | 2018 HD1 | HIS | S | 709 | 16.059 | 52.572 | 38.767 | 1.00 | 0.00 |
| ATOM | 2019 N | ASN | S | 710 | 19.990 | 53.954 | 38.905 | 1.00 | 0.00 |
| ATOM | 2020 CA | ASN | S | 710 | 19.992 | 55.150 | 38.053 | 1.00 | 0.00 |
| ATOM | 2021 C | ASN | S | 710 | 18.692 | 55.937 | 38.092 | 1.00 | 0.00 |
| ATOM | 2022 O | ASN | S | 710 | 18.677 | 57.152 | 38.327 | 1.00 | 0.00 |
| ATOM | 2023 CB | ASN | S | 710 | 20.370 | 54.756 | 36.610 | 1.00 | 0.00 |
| ATOM | 2024 CG | ASN | S | 710 | 20.278 | 55.926 | 35.633 | 1.00 | 0.00 |
| ATOM | 2025 OD1 | ASN | S | 710 | 20.397 | 57.103 | 35.980 | 1.00 | 0.00 |
| ATOM | 2026 ND2 | ASN | S | 710 | 19.987 | 55.554 | 34.380 | 1.00 | 0.00 |
| ATOM | 2027 H | ASN | S | 710 | 20.552 | 53.167 | 38.654 | 1.00 | 0.00 |
| ATOM | 2028 1HD2 | ASN | S | 710 | 19.801 | 56.232 | 33.667 | 1.00 | 0.00 |
| ATOM | 2029 2HD2 | ASN | S | 710 | 20.005 | 54.598 | 34.089 | 1.00 | 0.00 |
| ATOM | 2030 N | TYR | S | 711 | 17.605 | 55.171 | 37.875 | 1.00 | 0.00 |
| ATOM | 2031 CA | TYR | S | 711 | 16.318 | 55.849 | 38.858 | 1.00 | 0.00 |
| ATOM | 2032 C | TYR | S | 711 | 15.808 | 56.388 | 39.173 | 1.00 | 0.00 |
| ATOM | 2033 O | TYR | S | 711 | 15.246 | 57.473 | 39.182 | 1.00 | 0.00 |
| ATOM | 2034 CB | TYR | S | 711 | 15.245 | 55.072 | 37.096 | 1.00 | 0.00 |
| ATOM | 2035 CG | TYR | S | 711 | 15.018 | 55.772 | 35.775 | 1.00 | 0.00 |
| ATOM | 2036 CD1 | TYR | S | 711 | 15.630 | 55.257 | 34.614 | 1.00 | 0.00 |
| ATOM | 2037 CD2 | TYR | S | 711 | 14.217 | 56.933 | 35.741 | 1.00 | 0.00 |
| ATOM | 2038 CE1 | TYR | S | 711 | 15.456 | 55.934 | 33.396 | 1.00 | 0.00 |
| ATOM | 2039 CE2 | TYR | S | 711 | 14.048 | 57.613 | 34.523 | 1.00 | 0.00 |
| ATOM | 2040 CZ | TYR | S | 711 | 14.677 | 57.110 | 33.367 | 1.00 | 0.00 |
| ATOM | 2041 OH | TYR | S | 711 | 14.535 | 57.787 | 32.167 | 1.00 | 0.00 |
| ATOM | 2042 H | TYR | S | 711 | 17.691 | 54.184 | 37.751 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2043 HH | TYR | S | 711 | 14.815 | 57.204 | 31.457 | 1.00 | 0.00 |
| ATOM | 2044 N | GLU | S | 712 | 16.071 | 55.666 | 40.278 | 1.00 | 0.00 |
| ATOM | 2045 CA | GLU | S | 712 | 15.760 | 56.258 | 41.589 | 1.00 | 0.00 |
| ATOM | 2046 C | GLU | S | 712 | 16.455 | 57.591 | 41.791 | 1.00 | 0.00 |
| ATOM | 2047 O | GLU | S | 712 | 15.854 | 58.644 | 41.961 | 1.00 | 0.00 |
| ATOM | 2048 CB | GLU | S | 712 | 16.196 | 55.360 | 42.734 | 1.00 | 0.00 |
| ATOM | 2049 CG | GLU | S | 712 | 15.772 | 53.902 | 42.650 | 1.00 | 0.00 |
| ATOM | 2050 CD | GLU | S | 712 | 16.325 | 53.248 | 43.889 | 1.00 | 0.00 |
| ATOM | 2051 OE1 | GLU | S | 712 | 17.295 | 52.505 | 43.808 | 1.00 | 0.00 |
| ATOM | 2052 OE2 | GLU | S | 712 | 15.805 | 53.505 | 44.963 | 1.00 | 0.00 |
| ATOM | 2053 H | GLU | S | 712 | 16.604 | 54.826 | 40.246 | 1.00 | 0.00 |
| ATOM | 2054 N | SER | S | 713 | 17.794 | 57.510 | 41.633 | 1.00 | 0.00 |
| ATOM | 2055 CA | SER | S | 713 | 18.616 | 58.731 | 41.666 | 1.00 | 0.00 |
| ATOM | 2056 C | SER | S | 713 | 18.030 | 59.862 | 40.824 | 1.00 | 0.00 |
| ATOM | 2057 O | SER | S | 713 | 17.829 | 60.995 | 41.252 | 1.00 | 0.00 |
| ATOM | 2058 CB | SER | S | 713 | 20.045 | 58.363 | 41.253 | 1.00 | 0.00 |
| ATOM | 2059 OG | SER | S | 713 | 20.994 | 59.406 | 41.511 | 1.00 | 0.00 |
| ATOM | 2060 H | SER | S | 713 | 18.179 | 56.587 | 41.548 | 1.00 | 0.00 |
| ATOM | 2061 HG | SER | S | 713 | 20.838 | 59.728 | 42.403 | 1.00 | 0.00 |
| ATOM | 2062 N | ALA | S | 714 | 17.631 | 59.430 | 39.619 | 1.00 | 0.00 |
| ATOM | 2063 CA | ALA | S | 714 | 16.939 | 60.343 | 38.725 | 1.00 | 0.00 |
| ATOM | 2064 C | ALA | S | 714 | 15.644 | 60.928 | 39.253 | 1.00 | 0.00 |
| ATOM | 2065 O | ALA | S | 714 | 15.402 | 62.121 | 39.127 | 1.00 | 0.00 |
| ATOM | 2066 CB | ALA | S | 714 | 16.670 | 59.679 | 37.371 | 1.00 | 0.00 |
| ATOM | 2067 H | ALA | S | 714 | 17.691 | 58.456 | 39.419 | 1.00 | 0.00 |
| ATOM | 2068 N | ALA | S | 715 | 14.826 | 60.040 | 39.823 | 1.00 | 0.00 |
| ATOM | 2069 CA | ALA | S | 715 | 13.465 | 60.383 | 40.208 | 1.00 | 0.00 |
| ATOM | 2070 C | ALA | S | 715 | 13.366 | 61.174 | 41.490 | 1.00 | 0.00 |
| ATOM | 2071 O | ALA | S | 715 | 12.321 | 61.733 | 41.809 | 1.00 | 0.00 |
| ATOM | 2072 CB | ALA | S | 715 | 12.609 | 59.124 | 30.343 | 1.00 | 0.00 |
| ATOM | 2073 H | ALA | S | 715 | 15.206 | 59.145 | 40.048 | 1.00 | 0.00 |
| ATOM | 2074 N | GLU | S | 716 | 14.485 | 61.230 | 42.213 | 1.00 | 0.00 |
| ATOM | 2075 CA | GLU | S | 716 | 14.484 | 62.263 | 43.236 | 1.00 | 0.00 |
| ATOM | 2076 C | GLU | S | 716 | 15.170 | 63.535 | 42.802 | 1.00 | 0.00 |
| ATOM | 2077 O | GLU | S | 716 | 15.009 | 64.576 | 43.421 | 1.00 | 0.00 |
| ATOM | 2078 CB | GLU | S | 716 | 15.097 | 61.794 | 44.537 | 1.00 | 0.00 |
| ATOM | 2079 CG | GLU | S | 716 | 14.230 | 60.903 | 45.416 | 1.00 | 0.00 |
| ATOM | 2080 CD | GLU | S | 716 | 15.075 | 60.524 | 46.612 | 1.00 | 0.00 |
| ATOM | 2081 OE1 | GLU | S | 716 | 15.429 | 61.388 | 47.409 | 1.00 | 0.00 |
| ATOM | 2082 OE2 | GLU | S | 716 | 15.431 | 59.362 | 46.739 | 1.00 | 0.00 |
| ATOM | 2083 H | GLU | S | 716 | 15.281 | 60.645 | 42.043 | 1.00 | 0.00 |
| ATOM | 2084 N | ALA | S | 717 | 15.927 | 63.447 | 41.704 | 1.00 | 0.00 |
| ATOM | 2085 CA | ALA | S | 717 | 16.518 | 64.667 | 41.171 | 1.00 | 0.00 |
| ATOM | 2086 C | ALA | S | 717 | 15.497 | 65.553 | 40.471 | 1.00 | 0.00 |
| ATOM | 2087 O | ALA | S | 717 | 15.482 | 66.783 | 40.544 | 1.00 | 0.00 |
| ATOM | 2088 CB | ALA | S | 717 | 17.636 | 64.294 | 40.209 | 1.00 | 0.00 |
| ATOM | 2089 H | ALA | S | 717 | 16.044 | 62.581 | 41.221 | 1.00 | 0.00 |
| ATOM | 2090 N | ILE | S | 718 | 14.556 | 64.864 | 39.818 | 1.00 | 0.00 |
| ATOM | 2091 CA | ILE | S | 718 | 13.371 | 65.602 | 39.375 | 1.00 | 0.00 |
| ATOM | 2092 C | ILE | S | 718 | 12.576 | 66.288 | 40.504 | 1.00 | 0.00 |
| ATOM | 2093 O | ILE | S | 718 | 11.748 | 67.163 | 40.301 | 1.00 | 0.00 |
| ATOM | 2094 CB | ILE | S | 718 | 12.514 | 64.719 | 38.452 | 1.00 | 0.00 |
| ATOM | 2095 CG1 | ILE | S | 718 | 11.603 | 65.553 | 37.546 | 1.00 | 0.00 |
| ATOM | 2096 CG2 | ILE | S | 718 | 11.717 | 63.682 | 39.251 | 1.00 | 0.00 |
| ATOM | 2097 CD1 | ILE | S | 718 | 10.894 | 64.716 | 36.479 | 1.00 | 0.00 |
| ATOM | 2098 H | ILE | S | 718 | 14.627 | 63.870 | 39.736 | 1.00 | 0.00 |
| ATOM | 2099 N | GLN | S | 719 | 12.923 | 65.902 | 41.746 | 1.00 | 0.00 |
| ATOM | 2100 CA | GLN | S | 719 | 12.446 | 66.632 | 42.929 | 1.00 | 0.00 |
| ATOM | 2101 C | GLN | S | 719 | 13.503 | 67.525 | 43.578 | 1.00 | 0.00 |
| ATOM | 2102 O | GLN | S | 719 | 13.223 | 68.406 | 44.368 | 1.00 | 0.00 |
| ATOM | 2103 CB | GLN | S | 719 | 11.923 | 65.654 | 43.976 | 1.00 | 0.00 |
| ATOM | 2104 CG | GLN | S | 719 | 10.931 | 64.652 | 43.399 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2105 CD | GLN | S | 719 | 10.515 | 63.690 | 44.485 | 1.00 | 0.00 |
| ATOM | 2106 OE1 | GLN | S | 719 | 9.831 | 64.039 | 45.439 | 1.00 | 0.00 |
| ATOM | 2107 NE2 | GLN | S | 719 | 10.896 | 62.439 | 44.260 | 1.00 | 0.00 |
| ATOM | 2108 H | GLN | S | 719 | 13.601 | 65.171 | 41.850 | 1.00 | 0.00 |
| ATOM | 2109 1HE2 | GLN | S | 719 | 10.673 | 61.761 | 44.959 | 1.00 | 0.00 |
| ATOM | 2110 2HE2 | GLN | S | 719 | 11.381 | 62.222 | 43.416 | 1.00 | 0.00 |
| ATOM | 2111 N | ALA | S | 720 | 14.762 | 67.251 | 43.187 | 1.00 | 0.00 |
| ATOM | 2112 CA | ALA | S | 720 | 15.967 | 67.809 | 43.819 | 1.00 | 0.00 |
| ATOM | 2113 C | ALA | S | 720 | 16.199 | 67.335 | 45.247 | 1.00 | 0.00 |
| ATOM | 2114 O | ALA | S | 720 | 16.154 | 68.083 | 46.217 | 1.00 | 0.00 |
| ATOM | 2115 CB | ALA | S | 720 | 16.037 | 69.342 | 43.732 | 1.00 | 0.00 |
| ATOM | 2116 H | ALA | S | 720 | 14.909 | 66.440 | 42.625 | 1.00 | 0.00 |
| ATOM | 2117 N | VAL | S | 721 | 16.419 | 66.014 | 45.348 | 1.00 | 0.00 |
| ATOM | 2118 CA | VAL | S | 721 | 16.824 | 65.438 | 46.634 | 1.00 | 0.00 |
| ATOM | 2119 C | VAL | S | 721 | 18.030 | 64.523 | 46.466 | 1.00 | 0.00 |
| ATOM | 2120 O | VAL | S | 721 | 19.051 | 64.610 | 47.147 | 1.00 | 0.00 |
| ATOM | 2121 CB | VAL | S | 721 | 15.680 | 64.673 | 47.326 | 1.00 | 0.00 |
| ATOM | 2122 CG1 | VAL | S | 721 | 16.056 | 64.366 | 48.780 | 1.00 | 0.00 |
| ATOM | 2123 CG2 | VAL | S | 721 | 14.325 | 65.382 | 47.246 | 1.00 | 0.00 |
| ATOM | 2124 H | VAL | S | 721 | 16.325 | 65.466 | 44.521 | 1.00 | 0.00 |
| ATOM | 2125 N | ARG | S | 722 | 17.886 | 63.623 | 45.473 | 1.00 | 0.00 |
| ATOM | 2126 CA | ARG | S | 722 | 19.134 | 63.064 | 44.963 | 1.00 | 0.00 |
| ATOM | 2127 C | ARG | S | 722 | 19.823 | 64.129 | 44.136 | 1.00 | 0.00 |
| ATOM | 2128 O | ARG | S | 722 | 19.408 | 64.503 | 43.040 | 1.00 | 0.00 |
| ATOM | 2129 CB | ARG | S | 722 | 18.956 | 61.773 | 44.159 | 1.00 | 0.00 |
| ATOM | 2130 CG | ARG | S | 722 | 18.375 | 60.544 | 44.872 | 1.00 | 0.00 |
| ATOM | 2131 CD | ARG | S | 722 | 19.020 | 60.121 | 46.193 | 1.00 | 0.00 |
| ATOM | 2132 NE | ARG | S | 722 | 18.062 | 60.316 | 47.276 | 1.00 | 0.00 |
| ATOM | 2133 CZ | ARG | S | 722 | 17.894 | 59.523 | 48.355 | 1.00 | 0.00 |
| ATOM | 2134 NH1 | ARG | S | 722 | 16.909 | 59.813 | 49.198 | 1.00 | 0.00 |
| ATOM | 2135 NH2 | ARG | S | 722 | 18.673 | 58.465 | 48.557 | 1.00 | 0.00 |
| ATOM | 2136 H | ARG | S | 722 | 17.037 | 63.624 | 44.949 | 1.00 | 0.00 |
| ATOM | 2137 HE | ARG | S | 722 | 17.341 | 61.000 | 47.116 | 1.00 | 0.00 |
| ATOM | 2138 1HH1 | ARG | S | 722 | 16.815 | 59.374 | 50.088 | 1.00 | 0.00 |
| ATOM | 2139 2HH1 | ARG | S | 722 | 16.190 | 60.475 | 48.935 | 1.00 | 0.00 |
| ATOM | 2140 1HH2 | ARG | S | 722 | 18.567 | 57.944 | 49.404 | 1.00 | 0.00 |
| ATOM | 2141 2HH2 | ARG | S | 722 | 19.342 | 58.125 | 47.887 | 1.00 | 0.00 |
| ATOM | 2142 N | ASP | S | 723 | 20.836 | 64.653 | 44.826 | 1.00 | 0.00 |
| ATOM | 2143 CA | ASP | S | 723 | 21.174 | 66.025 | 44.529 | 1.00 | 0.00 |
| ATOM | 2144 C | ASP | S | 723 | 21.957 | 66.255 | 43.257 | 1.00 | 0.00 |
| ATOM | 2145 O | ASP | S | 723 | 21.368 | 66.398 | 42.182 | 1.00 | 0.00 |
| ATOM | 2146 CB | ASP | S | 723 | 21.786 | 66.617 | 45.788 | 1.00 | 0.00 |
| ATOM | 2147 CG | ASP | S | 723 | 21.603 | 68.105 | 45.856 | 1.00 | 0.00 |
| ATOM | 2148 OD1 | ASP | S | 723 | 20.668 | 68.618 | 45.246 | 1.00 | 0.00 |
| ATOM | 2149 OD2 | ASP | S | 723 | 22.395 | 68.740 | 46.538 | 1.00 | 0.00 |
| ATOM | 2150 H | ASP | S | 723 | 21.125 | 64.268 | 45.702 | 1.00 | 0.00 |
| ATOM | 2151 N | ASN | S | 724 | 23.285 | 66.304 | 43.384 | 1.00 | 0.00 |
| ATOM | 2152 CA | ASN | S | 724 | 23.954 | 66.403 | 42.100 | 1.00 | 0.00 |
| ATOM | 2153 C | ASN | S | 724 | 24.037 | 65.104 | 41.344 | 1.00 | 0.00 |
| ATOM | 2154 O | ASN | S | 724 | 24.516 | 64.063 | 41.789 | 1.00 | 0.00 |
| ATOM | 2155 CB | ASN | S | 724 | 25.285 | 67.146 | 42.147 | 1.00 | 0.00 |
| ATOM | 2156 CG | ASN | S | 724 | 25.626 | 67.602 | 40.736 | 1.00 | 0.00 |
| ATOM | 2157 OD1 | ASN | S | 724 | 26.754 | 67.470 | 40.276 | 1.00 | 0.00 |
| ATOM | 2158 ND2 | ASN | S | 724 | 24.603 | 68.097 | 40.032 | 1.00 | 0.00 |
| ATOM | 2159 H | ASN | S | 724 | 23.735 | 66.338 | 44.264 | 1.00 | 0.00 |
| ATOM | 2160 1HD2 | ASN | S | 724 | 24.676 | 68.413 | 39.085 | 1.00 | 0.00 |
| ATOM | 2161 2HD2 | ASN | S | 724 | 23.707 | 68.287 | 40.452 | 1.00 | 0.00 |
| ATOM | 2162 N | LYS | S | 725 | 23.489 | 65.226 | 40.148 | 1.00 | 0.00 |
| ATOM | 2163 CA | LYS | S | 725 | 23.140 | 64.043 | 39.392 | 1.00 | 0.00 |
| ATOM | 2164 C | LYS | S | 725 | 24.240 | 63.485 | 38.508 | 1.00 | 0.00 |
| ATOM | 2165 O | LYS | S | 725 | 24.077 | 63.405 | 37.291 | 1.00 | 0.00 |
| ATOM | 2166 CB | LYS | S | 725 | 21.867 | 64.407 | 38.631 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2167 CG | LYS | S | 725 | 21.082 | 63.256 | 38.028 | 1.00 | 0.00 |
| ATOM | 2168 CD | LYS | S | 725 | 19.780 | 63.741 | 37.413 | 1.00 | 0.00 |
| ATOM | 2169 CE | LYS | S | 725 | 18.980 | 62.591 | 36.843 | 1.00 | 0.00 |
| ATOM | 2170 NZ | LYS | S | 725 | 17.555 | 62.902 | 36.913 | 1.00 | 0.00 |
| ATOM | 2171 H | LYS | S | 725 | 23.158 | 66.115 | 39.835 | 1.00 | 0.00 |
| ATOM | 2172 1HZ | LYS | S | 725 | 17.066 | 62.431 | 36.129 | 1.00 | 0.00 |
| ATOM | 2173 2HZ | LYS | S | 725 | 17.095 | 62.675 | 37.811 | 1.00 | 0.00 |
| ATOM | 2174 3HZ | LYS | S | 725 | 17.413 | 63.901 | 36.693 | 1.00 | 0.00 |
| ATOM | 2175 N | LEU | S | 726 | 25.352 | 63.066 | 39.126 | 1.00 | 0.00 |
| ATOM | 2176 CA | LEU | S | 726 | 26.448 | 62.665 | 38.234 | 1.00 | 0.00 |
| ATOM | 2177 C | LEU | S | 726 | 26.383 | 61.267 | 37.633 | 1.00 | 0.00 |
| ATOM | 2178 O | LEU | S | 726 | 26.087 | 60.251 | 38.285 | 1.00 | 0.00 |
| ATOM | 2179 CB | LEU | S | 726 | 27.833 | 62.909 | 38.853 | 1.00 | 0.00 |
| ATOM | 2180 CG | LEU | S | 726 | 28.126 | 64.347 | 39.298 | 1.00 | 0.00 |
| ATOM | 2181 CD1 | LEU | S | 726 | 27.684 | 64.597 | 40.730 | 1.00 | 0.00 |
| ATOM | 2182 CD2 | LEU | S | 726 | 29.596 | 64.728 | 39.148 | 1.00 | 0.00 |
| ATOM | 2183 H | LEU | S | 726 | 25.506 | 63.299 | 40.089 | 1.00 | 0.00 |
| ATOM | 2184 N | HIS | S | 727 | 26.706 | 61.245 | 36.313 | 1.00 | 0.00 |
| ATOM | 2185 CA | HIS | S | 727 | 26.942 | 59.974 | 35.614 | 1.00 | 0.00 |
| ATOM | 2186 C | HIS | S | 727 | 27.794 | 60.102 | 34.345 | 1.00 | 0.00 |
| ATOM | 2187 O | HIS | S | 727 | 28.917 | 60.608 | 34.393 | 1.00 | 0.00 |
| ATOM | 2188 CB | HIS | S | 727 | 25.618 | 59.215 | 35.423 | 1.00 | 0.00 |
| ATOM | 2189 CG | HIS | S | 727 | 25.770 | 57.768 | 34.994 | 1.00 | 0.00 |
| ATOM | 2190 ND1 | HIS | S | 727 | 24.854 | 57.157 | 34.226 | 1.00 | 0.00 |
| ATOM | 2191 CD2 | HIS | S | 727 | 26.786 | 56.850 | 35.278 | 1.00 | 0.00 |
| ATOM | 2192 CE1 | HIS | S | 727 | 25.257 | 55.870 | 34.012 | 1.00 | 0.00 |
| ATOM | 2193 NE2 | HIS | S | 727 | 26.452 | 55.688 | 34.658 | 1.00 | 0.00 |
| ATOM | 2194 H | HIS | S | 727 | 26.685 | 62.119 | 35.823 | 1.00 | 0.00 |
| ATOM | 2195 HD1 | HIS | S | 727 | 24.008 | 57.573 | 33.939 | 1.00 | 0.00 |
| ATOM | 2196 N | ALA | S | 728 | 27.310 | 59.561 | 33.216 | 1.00 | 0.00 |
| ATOM | 2197 CA | ALA | S | 728 | 28.296 | 59.354 | 32.163 | 1.00 | 0.00 |
| ATOM | 2198 C | ALA | S | 728 | 27.789 | 59.711 | 30.791 | 1.00 | 0.00 |
| ATOM | 2199 O | ALA | S | 728 | 27.889 | 58.912 | 29.856 | 1.00 | 0.00 |
| ATOM | 2200 CB | ALA | S | 728 | 28.792 | 57.903 | 32.166 | 1.00 | 0.00 |
| ATOM | 2201 H | ALA | S | 728 | 26.335 | 59.410 | 33.039 | 1.00 | 0.00 |
| ATOM | 2202 N | PHE | S | 729 | 27.276 | 60.956 | 30.723 | 1.00 | 0.00 |
| ATOM | 2203 CA | PHE | S | 729 | 26.605 | 61.427 | 29.511 | 1.00 | 0.00 |
| ATOM | 2204 C | PHE | S | 729 | 25.334 | 60.668 | 29.141 | 1.00 | 0.00 |
| ATOM | 2205 O | PHE | S | 729 | 24.937 | 59.661 | 29.732 | 1.00 | 0.00 |
| ATOM | 2206 CB | PHE | S | 729 | 27.572 | 61.497 | 28.309 | 1.00 | 0.00 |
| ATOM | 2207 CG | PHE | S | 729 | 28.286 | 62.828 | 28.191 | 1.00 | 0.00 |
| ATOM | 2208 CD1 | PHE | S | 729 | 28.365 | 63.427 | 26.915 | 1.00 | 0.00 |
| ATOM | 2209 CD2 | PHE | S | 729 | 28.868 | 63.449 | 29.320 | 1.00 | 0.00 |
| ATOM | 2210 CE1 | PHE | S | 729 | 29.035 | 64.656 | 26.761 | 1.00 | 0.00 |
| ATOM | 2211 CE2 | PHE | S | 729 | 29.533 | 64.681 | 29.167 | 1.00 | 0.00 |
| ATOM | 2212 CZ | PHE | S | 729 | 29.612 | 65.272 | 27.890 | 1.00 | 0.00 |
| ATOM | 2213 H | PHE | S | 729 | 27.312 | 61.512 | 31.555 | 1.00 | 0.00 |
| ATOM | 2214 N | ILE | S | 730 | 24.714 | 61.215 | 28.090 | 1.00 | 0.00 |
| ATOM | 2215 CA | ILE | S | 730 | 23.459 | 60.778 | 27.476 | 1.00 | 0.00 |
| ATOM | 2216 C | ILE | S | 730 | 22.319 | 60.313 | 28.392 | 1.00 | 0.00 |
| ATOM | 2217 O | ILE | S | 730 | 21.387 | 61.081 | 28.633 | 1.00 | 0.00 |
| ATOM | 2218 CB | ILE | S | 730 | 23.742 | 59.960 | 26.195 | 1.00 | 0.00 |
| ATOM | 2219 CG1 | ILE | S | 730 | 22.509 | 59.797 | 25.311 | 1.00 | 0.00 |
| ATOM | 2220 CG2 | ILE | S | 730 | 24.440 | 58.616 | 26.444 | 1.00 | 0.00 |
| ATOM | 2221 CD1 | ILE | S | 730 | 22.870 | 59.438 | 23.867 | 1.00 | 0.00 |
| ATOM | 2222 H | ILE | S | 730 | 25.109 | 62.087 | 27.799 | 1.00 | 0.00 |
| ATOM | 2223 N | TRP | S | 731 | 22.452 | 59.093 | 28.969 | 1.00 | 0.00 |
| ATOM | 2224 CA | TRP | S | 731 | 21.679 | 58.715 | 30.170 | 1.00 | 0.00 |
| ATOM | 2225 C | TRP | S | 731 | 21.472 | 59.848 | 31.167 | 1.00 | 0.00 |
| ATOM | 2226 O | TRP | S | 731 | 20.436 | 59.999 | 31.815 | 1.00 | 0.00 |
| ATOM | 2227 CB | TRP | S | 731 | 22.392 | 57.595 | 30.937 | 1.00 | 0.00 |
| ATOM | 2228 CG | TRP | S | 731 | 22.257 | 56.250 | 30.267 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2229 CD1 | TRP | S | 731 | 21.196 | 55.351 | 30.436 | 1.00 | 0.00 |
| ATOM | 2230 CD2 | TRP | S | 731 | 23.176 | 55.589 | 29.369 | 1.00 | 0.00 |
| ATOM | 2231 NE1 | TRP | S | 731 | 21.394 | 54.211 | 29.721 | 1.00 | 0.00 |
| ATOM | 2232 CE2 | TRP | S | 731 | 22.605 | 54.312 | 29.045 | 1.00 | 0.00 |
| ATOM | 2233 CE3 | TRP | S | 731 | 24.423 | 55.962 | 28.822 | 1.00 | 0.00 |
| ATOM | 2234 CZ2 | TRP | S | 731 | 23.292 | 53.436 | 28.178 | 1.00 | 0.00 |
| ATOM | 2235 CZ3 | TRP | S | 731 | 25.100 | 55.075 | 27.958 | 1.00 | 0.00 |
| ATOM | 2236 CH2 | TRP | S | 731 | 24.537 | 53.821 | 27.639 | 1.00 | 0.00 |
| ATOM | 2237 H | TRP | S | 731 | 23.222 | 58.826 | 28.684 | 1.00 | 0.00 |
| ATOM | 2238 HE1 | TRP | S | 731 | 20.756 | 53.467 | 29.682 | 1.00 | 0.00 |
| ATOM | 2239 N | ASP | S | 732 | 22.539 | 60.649 | 31.236 | 1.00 | 0.00 |
| ATOM | 2240 CA | ASP | S | 732 | 22.588 | 61.774 | 32.145 | 1.00 | 0.00 |
| ATOM | 2241 C | ASP | S | 732 | 22.868 | 63.135 | 31.538 | 1.00 | 0.00 |
| ATOM | 2242 O | ASP | S | 732 | 22.570 | 64.180 | 32.121 | 1.00 | 0.00 |
| ATOM | 2243 CB | ASP | S | 732 | 23.516 | 61.398 | 33.283 | 1.00 | 0.00 |
| ATOM | 2244 CG | ASP | S | 732 | 22.646 | 60.810 | 34.365 | 1.00 | 0.00 |
| ATOM | 2245 OD1 | ASP | S | 732 | 22.000 | 61.572 | 35.054 | 1.00 | 0.00 |
| ATOM | 2246 OD2 | ASP | S | 732 | 22.574 | 59.599 | 34.540 | 1.00 | 0.00 |
| ATOM | 2247 H | ASP | S | 732 | 23.353 | 60.362 | 30.743 | 1.00 | 0.00 |
| ATOM | 2248 N | SER | S | 733 | 23.377 | 63.105 | 30.286 | 1.00 | 0.00 |
| ATOM | 2249 CA | SER | S | 733 | 23.289 | 64.350 | 29.518 | 1.00 | 0.00 |
| ATOM | 2250 C | SER | S | 733 | 22.223 | 64.364 | 28.418 | 1.00 | 0.00 |
| ATOM | 2251 O | SER | S | 733 | 21.088 | 64.732 | 28.688 | 1.00 | 0.00 |
| ATOM | 2252 CB | SER | S | 733 | 24.665 | 64.830 | 29.046 | 1.00 | 0.00 |
| ATOM | 2253 OG | SER | S | 733 | 25.227 | 63.934 | 28.072 | 1.00 | 0.00 |
| ATOM | 2254 H | SER | S | 733 | 23.647 | 62.253 | 29.851 | 1.00 | 0.00 |
| ATOM | 2255 HG | SER | S | 733 | 25.868 | 64.482 | 27.614 | 1.00 | 0.00 |
| ATOM | 2256 N | ALA | S | 734 | 22.573 | 63.960 | 27.180 | 1.00 | 0.00 |
| ATOM | 2257 CA | ALA | S | 734 | 21.705 | 64.195 | 26.015 | 1.00 | 0.00 |
| ATOM | 2258 C | ALA | S | 734 | 20.192 | 63.958 | 26.096 | 1.00 | 0.00 |
| ATOM | 2259 O | ALA | S | 734 | 19.412 | 64.716 | 25.528 | 1.00 | 0.00 |
| ATOM | 2260 CB | ALA | S | 734 | 22.255 | 63.479 | 24.781 | 1.00 | 0.00 |
| ATOM | 2261 H | ALA | S | 734 | 23.507 | 63.640 | 27.020 | 1.00 | 0.00 |
| ATOM | 2262 N | VAL | S | 735 | 19.774 | 62.927 | 26.850 | 1.00 | 0.00 |
| ATOM | 2263 CA | VAL | S | 735 | 18.323 | 62.708 | 26.910 | 1.00 | 0.00 |
| ATOM | 2264 C | VAL | S | 735 | 17.755 | 62.999 | 28.297 | 1.00 | 0.00 |
| ATOM | 2265 O | VAL | S | 735 | 17.044 | 62.227 | 28.932 | 1.00 | 0.00 |
| ATOM | 2266 CB | VAL | S | 735 | 17.950 | 61.298 | 26.409 | 1.00 | 0.00 |
| ATOM | 2267 CG1 | VAL | S | 735 | 16.453 | 61.184 | 26.099 | 1.00 | 0.00 |
| ATOM | 2268 CG2 | VAL | S | 735 | 18.764 | 60.900 | 25.173 | 1.00 | 0.00 |
| ATOM | 2269 H | VAL | S | 735 | 20.415 | 62.332 | 27.337 | 1.00 | 0.00 |
| ATOM | 2270 N | LEU | S | 736 | 18.152 | 64.168 | 28.806 | 1.00 | 0.00 |
| ATOM | 2271 CA | LEU | S | 736 | 17.820 | 64.394 | 30.211 | 1.00 | 0.00 |
| ATOM | 2272 C | LEU | S | 736 | 16.861 | 65.546 | 30.445 | 1.00 | 0.00 |
| ATOM | 2273 O | LEU | S | 736 | 16.921 | 66.565 | 29.768 | 1.00 | 0.00 |
| ATOM | 2274 CB | LEU | S | 736 | 19.104 | 64.543 | 31.033 | 1.00 | 0.00 |
| ATOM | 2275 CG | LEU | S | 736 | 18.878 | 64.625 | 32.540 | 1.00 | 0.00 |
| ATOM | 2276 CD1 | LEU | S | 736 | 19.642 | 63.548 | 33.297 | 1.00 | 0.00 |
| ATOM | 2277 CD2 | LEU | S | 736 | 19.082 | 66.043 | 33.075 | 1.00 | 0.00 |
| ATOM | 2278 H | LEU | S | 736 | 18.653 | 64.868 | 28.291 | 1.00 | 0.00 |
| ATOM | 2279 N | GLU | S | 737 | 15.990 | 65.285 | 31.439 | 1.00 | 0.00 |
| ATOM | 2280 CA | GLU | S | 737 | 15.025 | 66.217 | 32.050 | 1.00 | 0.00 |
| ATOM | 2281 C | GLU | S | 737 | 15.095 | 67.728 | 31.746 | 1.00 | 0.00 |
| ATOM | 2282 O | GLU | S | 737 | 15.436 | 68.565 | 32.586 | 1.00 | 0.00 |
| ATOM | 2283 CB | GLU | S | 737 | 14.978 | 65.958 | 33.571 | 1.00 | 0.00 |
| ATOM | 2284 CG | GLU | S | 737 | 14.798 | 64.485 | 34.013 | 1.00 | 0.00 |
| ATOM | 2285 CD | GLU | S | 737 | 16.092 | 63.850 | 34.528 | 1.00 | 0.00 |
| ATOM | 2286 OE1 | GLU | S | 737 | 16.319 | 62.658 | 34.351 | 1.00 | 0.00 |
| ATOM | 2287 OE2 | GLU | S | 737 | 16.902 | 64.522 | 35.144 | 1.00 | 0.00 |
| ATOM | 2288 H | GLU | S | 737 | 16.007 | 64.323 | 31.713 | 1.00 | 0.00 |
| ATOM | 2289 N | PHE | S | 738 | 14.685 | 68.038 | 30.502 | 1.00 | 0.00 |
| ATOM | 2290 CA | PHE | S | 738 | 14.931 | 69.323 | 29.827 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2291 C | PHE | S | 738 | 14.658 | 70.671 | 30.492 | 1.00 | 0.00 |
| ATOM | 2292 O | PHE | S | 738 | 15.576 | 71.472 | 30.642 | 1.00 | 0.00 |
| ATOM | 2293 CB | PHE | S | 738 | 14.359 | 69.280 | 28.404 | 1.00 | 0.00 |
| ATOM | 2294 CG | PHE | S | 738 | 15.061 | 68.193 | 27.616 | 1.00 | 0.00 |
| ATOM | 2295 CD1 | PHE | S | 738 | 16.364 | 68.426 | 27.122 | 1.00 | 0.00 |
| ATOM | 2296 CD2 | PHE | S | 738 | 14.412 | 66.956 | 27.403 | 1.00 | 0.00 |
| ATOM | 2297 CE1 | PHE | S | 738 | 17.035 | 67.402 | 29.425 | 1.00 | 0.00 |
| ATOM | 2298 CE2 | PHE | S | 738 | 15.082 | 65.931 | 26.708 | 1.00 | 0.00 |
| ATOM | 2299 CZ | PHE | S | 738 | 16.391 | 66.162 | 26.233 | 1.00 | 0.00 |
| ATOM | 2300 H | PHE | S | 738 | 14.489 | 67.237 | 29.943 | 1.00 | 0.00 |
| ATOM | 2301 N | GLU | S | 739 | 13.409 | 70.929 | 30.919 | 1.00 | 0.00 |
| ATOM | 2302 CA | GLU | S | 739 | 13.105 | 72.315 | 31.315 | 1.00 | 0.00 |
| ATOM | 2303 C | GLU | S | 739 | 13.507 | 72.769 | 32.727 | 1.00 | 0.00 |
| ATOM | 2304 O | GLU | S | 739 | 12.778 | 73.447 | 33.451 | 1.00 | 0.00 |
| ATOM | 2305 CB | GLU | S | 739 | 11.632 | 72.615 | 31.015 | 1.00 | 0.00 |
| ATOM | 2306 CG | GLU | S | 739 | 11.352 | 74.077 | 30.639 | 1.00 | 0.00 |
| ATOM | 2307 CD | GLU | S | 739 | 12.054 | 74.443 | 29.342 | 1.00 | 0.00 |
| ATOM | 2308 OE1 | GLU | S | 739 | 12.862 | 75.367 | 29.344 | 1.00 | 0.00 |
| ATOM | 2309 OE2 | GLU | S | 739 | 11.786 | 73.813 | 28.324 | 1.00 | 0.00 |
| ATOM | 2310 H | GLU | S | 739 | 12.742 | 70.188 | 30.882 | 1.00 | 0.00 |
| ATOM | 2311 N | ALA | S | 740 | 14.721 | 72.335 | 33.115 | 1.00 | 0.00 |
| ATOM | 2312 CA | ALA | S | 740 | 15.225 | 72.574 | 34.469 | 1.00 | 0.00 |
| ATOM | 2313 C | ALA | S | 740 | 16.226 | 73.720 | 34.567 | 1.00 | 0.00 |
| ATOM | 2314 O | ALA | S | 740 | 17.359 | 73.592 | 35.027 | 1.00 | 0.00 |
| ATOM | 2315 CB | ALA | S | 740 | 15.848 | 71.290 | 35.019 | 1.00 | 0.00 |
| ATOM | 2316 H | ALA | S | 740 | 15.340 | 71.898 | 32.457 | 1.00 | 0.00 |
| ATOM | 2317 N | SER | S | 741 | 15.701 | 74.874 | 34.083 | 1.00 | 0.00 |
| ATOM | 2318 CA | SER | S | 741 | 16.420 | 76.150 | 34.200 | 1.00 | 0.00 |
| ATOM | 2319 C | SER | S | 741 | 17.805 | 76.185 | 33.584 | 1.00 | 0.00 |
| ATOM | 2320 O | SER | S | 741 | 18.738 | 76.799 | 34.090 | 1.00 | 0.00 |
| ATOM | 2321 CB | SER | S | 741 | 16.434 | 76.578 | 35.672 | 1.00 | 0.00 |
| ATOM | 2322 OG | SER | S | 741 | 15.121 | 76.306 | 36.200 | 1.00 | 0.00 |
| ATOM | 2323 H | SER | S | 741 | 14.755 | 74.875 | 33.757 | 1.00 | 0.00 |
| ATOM | 2324 HG | SER | S | 741 | 15.235 | 75.944 | 37.081 | 1.00 | 0.00 |
| ATOM | 2325 N | GLN | S | 742 | 17.927 | 75.462 | 32.466 | 1.00 | 0.00 |
| ATOM | 2326 CA | GLN | S | 742 | 19.275 | 75.052 | 32.100 | 1.00 | 0.00 |
| ATOM | 2327 C | GLN | S | 742 | 20.252 | 76.136 | 31.715 | 1.00 | 0.00 |
| ATOM | 2328 O | GLN | S | 742 | 19.898 | 77.163 | 31.142 | 1.00 | 0.00 |
| ATOM | 2329 CB | GLN | S | 742 | 19.237 | 73.929 | 31.070 | 1.00 | 0.00 |
| ATOM | 2330 CG | GLN | S | 742 | 18.377 | 72.812 | 31.646 | 1.00 | 0.00 |
| ATOM | 2331 CD | GLN | S | 742 | 18.506 | 71.542 | 30.848 | 1.00 | 0.00 |
| ATOM | 2332 OE1 | GLN | S | 742 | 18.661 | 71.506 | 29.627 | 1.00 | 0.00 |
| ATOM | 2333 NE2 | GLN | S | 742 | 18.338 | 70.451 | 31.590 | 1.00 | 0.00 |
| ATOM | 2334 H | GLN | S | 742 | 17.121 | 75.120 | 31.982 | 1.00 | 0.00 |
| ATOM | 2335 1HE2 | GLN | S | 742 | 18.145 | 69.540 | 31.229 | 1.00 | 0.00 |
| ATOM | 2336 2HE2 | GLN | S | 742 | 18.498 | 70.549 | 32.852 | 1.00 | 0.00 |
| ATOM | 2337 N | LYS | S | 743 | 21.485 | 75.793 | 32.080 | 1.00 | 0.00 |
| ATOM | 2338 CA | LYS | S | 743 | 22.757 | 76.318 | 31.600 | 1.00 | 0.00 |
| ATOM | 2339 C | LYS | S | 743 | 23.796 | 75.561 | 32.396 | 1.00 | 0.00 |
| ATOM | 2340 O | LYS | S | 743 | 23.599 | 75.179 | 33.548 | 1.00 | 0.00 |
| ATOM | 2341 CB | LYS | S | 743 | 22.917 | 77.837 | 31.749 | 1.00 | 0.00 |
| ATOM | 2342 CG | LYS | S | 743 | 24.228 | 78.468 | 31.236 | 1.00 | 0.00 |
| ATOM | 2343 CD | LYS | S | 743 | 24.480 | 78.281 | 29.735 | 1.00 | 0.00 |
| ATOM | 2344 CE | LYS | S | 743 | 25.589 | 79.180 | 29.166 | 1.00 | 0.00 |
| ATOM | 2345 NZ | LYS | S | 743 | 26.933 | 78.806 | 29.622 | 1.00 | 0.00 |
| ATOM | 2346 H | LYS | S | 743 | 21.593 | 74.989 | 32.671 | 1.00 | 0.00 |
| ATOM | 2347 1HZ | LYS | S | 743 | 27.950 | 79.524 | 29.441 | 1.00 | 0.00 |
| ATOM | 2348 2HZ | LYS | S | 743 | 27.019 | 78.620 | 30.647 | 1.00 | 0.00 |
| ATOM | 2349 3HZ | LYS | S | 743 | 27.287 | 77.913 | 29.209 | 1.00 | 0.00 |
| ATOM | 2350 N | CYS | S | 744 | 24.893 | 75.291 | 31.708 | 1.00 | 0.00 |
| ATOM | 2351 CA | CYS | S | 744 | 25.741 | 74.270 | 32.278 | 1.00 | 0.00 |
| ATOM | 2352 C | CYS | S | 744 | 27.108 | 74.347 | 31.678 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2353 O | CYS | S | 744 | 27.313 | 73.925 | 30.543 | 1.00 | 0.00 |
| ATOM | 2354 CB | CYS | S | 744 | 25.123 | 72.919 | 31.958 | 1.00 | 0.00 |
| ATOM | 2355 SG | CYS | S | 744 | 25.853 | 71.516 | 32.822 | 1.00 | 0.00 |
| ATOM | 2356 H | CYS | S | 744 | 25.044 | 75.584 | 30.767 | 1.00 | 0.00 |
| ATOM | 2357 N | ASP | S | 745 | 28.027 | 74.846 | 32.499 | 1.00 | 0.00 |
| ATOM | 2358 CA | ASP | S | 745 | 29.419 | 74.922 | 32.056 | 1.00 | 0.00 |
| ATOM | 2359 C | ASP | S | 745 | 30.328 | 74.163 | 33.004 | 1.00 | 0.00 |
| ATOM | 2360 O | ASP | S | 745 | 31.554 | 74.299 | 33.044 | 1.00 | 0.00 |
| ATOM | 2361 CB | ASP | S | 745 | 29.832 | 76.403 | 31.957 | 1.00 | 0.00 |
| ATOM | 2362 CG | ASP | S | 745 | 28.733 | 77.234 | 31.302 | 1.00 | 0.00 |
| ATOM | 2363 OD1 | ASP | S | 745 | 28.127 | 76.790 | 30.340 | 1.00 | 0.00 |
| ATOM | 2364 OD2 | ASP | S | 745 | 28.432 | 78.330 | 31.750 | 1.00 | 0.00 |
| ATOM | 2365 H | ASP | S | 745 | 27.710 | 75.365 | 33.291 | 1.00 | 0.00 |
| ATOM | 2366 N | LEU | S | 746 | 29.613 | 73.428 | 33.863 | 1.00 | 0.00 |
| ATOM | 2367 CA | LEU | S | 746 | 30.253 | 72.993 | 35.090 | 1.00 | 0.00 |
| ATOM | 2368 C | LEU | S | 746 | 30.422 | 71.502 | 35.146 | 1.00 | 0.00 |
| ATOM | 2369 O | LEU | S | 746 | 30.692 | 70.916 | 36.193 | 1.00 | 0.00 |
| ATOM | 2370 CB | LEU | S | 746 | 29.473 | 73.490 | 36.307 | 1.00 | 0.00 |
| ATOM | 2371 CG | LEU | S | 746 | 29.418 | 75.013 | 36.441 | 1.00 | 0.00 |
| ATOM | 2372 CD1 | LEU | S | 746 | 28.493 | 75.435 | 37.582 | 1.00 | 0.00 |
| ATOM | 2373 CD2 | LEU | S | 746 | 30.811 | 75.634 | 36.575 | 1.00 | 0.00 |
| ATOM | 2374 H | LEU | S | 746 | 28.745 | 73.068 | 33.536 | 1.00 | 0.00 |
| ATOM | 2375 N | VAL | S | 747 | 30.267 | 70.379 | 33.978 | 1.00 | 0.00 |
| ATOM | 2376 CA | VAL | S | 747 | 30.552 | 69.449 | 34.002 | 1.00 | 0.00 |
| ATOM | 2377 C | VAL | S | 747 | 32.045 | 69.217 | 34.123 | 1.00 | 0.00 |
| ATOM | 2378 O | VAL | S | 747 | 32.872 | 69.979 | 33.620 | 1.00 | 0.00 |
| ATOM | 2379 CB | VAL | S | 747 | 29.863 | 68.834 | 32.791 | 1.00 | 0.00 |
| ATOM | 2380 CG1 | VAL | S | 747 | 30.264 | 67.426 | 32.388 | 1.00 | 0.00 |
| ATOM | 2381 CG2 | VAL | S | 747 | 28.384 | 68.945 | 33.102 | 1.00 | 0.00 |
| ATOM | 2382 H | VAL | S | 747 | 30.008 | 71.342 | 33.127 | 1.00 | 0.00 |
| ATOM | 2383 N | THR | S | 748 | 32.363 | 68.224 | 34.950 | 1.00 | 0.00 |
| ATOM | 2384 CA | THR | S | 748 | 33.537 | 68.394 | 35.792 | 1.00 | 0.00 |
| ATOM | 2385 C | THR | S | 748 | 34.774 | 67.666 | 35.345 | 1.00 | 0.00 |
| ATOM | 2386 O | THR | S | 748 | 34.777 | 66.441 | 35.229 | 1.00 | 0.00 |
| ATOM | 2387 CB | THR | S | 748 | 33.161 | 68.115 | 37.262 | 1.00 | 0.00 |
| ATOM | 2388 OG1 | THR | S | 748 | 34.268 | 68.335 | 38.148 | 1.00 | 0.00 |
| ATOM | 2389 CG2 | THR | S | 748 | 32.577 | 66.723 | 37.499 | 1.00 | 0.00 |
| ATOM | 2390 H | THR | S | 748 | 31.719 | 67.470 | 35.044 | 1.00 | 0.00 |
| ATOM | 2391 HG1 | THR | S | 748 | 34.390 | 69.284 | 38.057 | 1.00 | 0.00 |
| ATOM | 2392 N | THR | S | 749 | 35.818 | 68.483 | 35.106 | 1.00 | 0.00 |
| ATOM | 2393 CA | THR | S | 749 | 37.101 | 67.954 | 34.655 | 1.00 | 0.00 |
| ATOM | 2394 C | THR | S | 749 | 37.918 | 67.342 | 35.801 | 1.00 | 0.00 |
| ATOM | 2395 O | THR | S | 749 | 37.476 | 67.354 | 36.957 | 1.00 | 0.00 |
| ATOM | 2396 CB | THR | S | 749 | 37.854 | 69.053 | 33.878 | 1.00 | 0.00 |
| ATOM | 2397 OG1 | THR | S | 749 | 36.980 | 70.125 | 33.452 | 1.00 | 0.00 |
| ATOM | 2398 CG2 | THR | S | 749 | 38.570 | 68.468 | 32.656 | 1.00 | 0.00 |
| ATOM | 2399 H | THR | S | 749 | 35.736 | 69.466 | 35.286 | 1.00 | 0.00 |
| ATOM | 2400 HG1 | THR | S | 749 | 36.185 | 69.668 | 33.179 | 1.00 | 0.00 |
| ATOM | 2401 N | GLY | S | 750 | 39.092 | 66.779 | 35.468 | 1.00 | 0.00 |
| ATOM | 2402 CA | GLY | S | 750 | 39.764 | 65.916 | 36.436 | 1.00 | 0.00 |
| ATOM | 2403 C | GLY | S | 750 | 39.614 | 64.450 | 36.062 | 1.00 | 0.00 |
| ATOM | 2404 O | GLY | S | 750 | 39.134 | 63.604 | 36.821 | 1.00 | 0.00 |
| ATOM | 2405 H | GLY | S | 750 | 39.434 | 66.847 | 34.535 | 1.00 | 0.00 |
| ATOM | 2406 N | GLU | S | 751 | 40.016 | 64.189 | 34.813 | 1.00 | 0.00 |
| ATOM | 2407 CA | GLU | S | 751 | 39.911 | 62.844 | 34.238 | 1.00 | 0.00 |
| ATOM | 2408 C | GLU | S | 751 | 41.022 | 61.924 | 34.708 | 1.00 | 0.00 |
| ATOM | 2409 O | GLU | S | 751 | 42.167 | 62.362 | 34.835 | 1.00 | 0.00 |
| ATOM | 2410 CB | GLU | S | 751 | 39.398 | 62.898 | 32.702 | 1.00 | 0.00 |
| ATOM | 2411 CG | GLU | S | 751 | 39.032 | 64.016 | 32.106 | 1.00 | 0.00 |
| ATOM | 2412 CD | GLU | S | 751 | 38.039 | 63.477 | 31.088 | 1.00 | 0.00 |
| ATOM | 2413 OE1 | GLU | S | 751 | 38.053 | 63.915 | 29.942 | 1.00 | 0.00 |
| ATOM | 2414 OE2 | GLU | S | 751 | 37.216 | 62.640 | 31.448 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2415 H | GLU | S | 751 | 40.472 | 64.963 | 34.383 | 1.00 | 0.00 |
| ATOM | 2416 N | LEU | S | 752 | 40.595 | 60.668 | 34.979 | 1.00 | 0.00 |
| ATOM | 2417 CA | LEU | S | 752 | 41.362 | 59.517 | 35.487 | 1.00 | 0.00 |
| ATOM | 2418 C | LEU | S | 752 | 40.418 | 58.601 | 36.245 | 1.00 | 0.00 |
| ATOM | 2419 O | LEU | S | 752 | 40.122 | 57.471 | 35.856 | 1.00 | 0.00 |
| ATOM | 2420 CB | LEU | S | 752 | 42.547 | 59.875 | 36.402 | 1.00 | 0.00 |
| ATOM | 2421 CG | LEU | S | 752 | 43.405 | 58.674 | 36.819 | 1.00 | 0.00 |
| ATOM | 2422 CD1 | LEU | S | 752 | 44.032 | 57.962 | 35.618 | 1.00 | 0.00 |
| ATOM | 2423 CD2 | LEU | S | 752 | 44.447 | 59.064 | 37.868 | 1.00 | 0.00 |
| ATOM | 2424 H | LEU | S | 752 | 39.660 | 60.533 | 34.649 | 1.00 | 0.00 |
| ATOM | 2425 N | PHE | S | 753 | 39.893 | 59.202 | 37.325 | 1.00 | 0.00 |
| ATOM | 2426 CA | PHE | S | 753 | 38.810 | 58.542 | 38.040 | 1.00 | 0.00 |
| ATOM | 2427 C | PHE | S | 753 | 37.536 | 58.742 | 37.255 | 1.00 | 0.00 |
| ATOM | 2428 O | PHE | S | 753 | 36.826 | 57.797 | 36.909 | 1.00 | 0.00 |
| ATOM | 2429 CB | PHE | S | 753 | 38.671 | 59.086 | 39.457 | 1.00 | 0.00 |
| ATOM | 2430 CG | PHE | S | 753 | 39.850 | 58.694 | 40.315 | 1.00 | 0.00 |
| ATOM | 2431 CD1 | PHE | S | 753 | 40.953 | 59.569 | 40.427 | 1.00 | 0.00 |
| ATOM | 2432 CD2 | PHE | S | 753 | 39.822 | 57.460 | 41.001 | 1.00 | 0.00 |
| ATOM | 2433 CE1 | PHE | S | 753 | 42.044 | 59.205 | 41.239 | 1.00 | 0.00 |
| ATOM | 2434 CE2 | PHE | S | 753 | 40.912 | 57.096 | 41.815 | 1.00 | 0.00 |
| ATOM | 2435 CZ | PHE | S | 753 | 42.012 | 57.973 | 41.926 | 1.00 | 0.00 |
| ATOM | 2436 H | PHE | S | 753 | 40.125 | 60.160 | 37.498 | 1.00 | 0.00 |
| ATOM | 2437 N | PHE | S | 754 | 37.356 | 60.016 | 36.866 | 1.00 | 0.00 |
| ATOM | 2438 CA | PHE | S | 754 | 36.417 | 60.329 | 35.786 | 1.00 | 0.00 |
| ATOM | 2439 C | PHE | S | 754 | 36.807 | 59.534 | 34.565 | 1.00 | 0.00 |
| ATOM | 2440 O | PHE | S | 754 | 37.926 | 59.645 | 34.069 | 1.00 | 0.00 |
| ATOM | 2441 CB | PHE | S | 754 | 36.349 | 61.839 | 35.517 | 1.00 | 0.00 |
| ATOM | 2442 CG | PHE | S | 754 | 35.823 | 62.627 | 36.709 | 1.00 | 0.00 |
| ATOM | 2443 CD1 | PHE | S | 754 | 34.989 | 62.027 | 37.684 | 1.00 | 0.00 |
| ATOM | 2444 CD2 | PHE | S | 754 | 36.176 | 63.990 | 36.814 | 1.00 | 0.00 |
| ATOM | 2445 CE1 | PHE | S | 754 | 34.511 | 62.791 | 38.766 | 1.00 | 0.00 |
| ATOM | 2446 CE2 | PHE | S | 754 | 35.706 | 64.756 | 37.897 | 1.00 | 0.00 |
| ATOM | 2447 CZ | PHE | S | 754 | 34.878 | 64.148 | 38.863 | 1.00 | 0.00 |
| ATOM | 2448 H | PHE | S | 754 | 37.791 | 60.760 | 37.374 | 1.00 | 0.00 |
| ATOM | 2449 N | ARG | S | 755 | 35.904 | 58.582 | 34.251 | 1.00 | 0.00 |
| ATOM | 2450 CA | ARG | S | 755 | 36.334 | 57.466 | 33.396 | 1.00 | 0.00 |
| ATOM | 2451 C | ARG | S | 755 | 36.448 | 57.983 | 31.988 | 1.00 | 0.00 |
| ATOM | 2452 O | ARG | S | 755 | 35.449 | 58.349 | 31.378 | 1.00 | 0.00 |
| ATOM | 2453 CB | ARG | S | 755 | 35.342 | 56.301 | 33.442 | 1.00 | 0.00 |
| ATOM | 2454 CG | ARG | S | 755 | 35.798 | 55.038 | 34.181 | 1.00 | 0.00 |
| ATOM | 2455 CD | ARG | S | 755 | 35.726 | 55.093 | 35.705 | 1.00 | 0.00 |
| ATOM | 2456 NE | ARG | S | 755 | 36.413 | 53.954 | 36.312 | 1.00 | 0.00 |
| ATOM | 2457 CZ | ARG | S | 755 | 37.636 | 54.133 | 36.866 | 1.00 | 0.00 |
| ATOM | 2458 NH1 | ARG | S | 755 | 38.320 | 53.097 | 37.321 | 1.00 | 0.00 |
| ATOM | 2459 NH2 | ARG | S | 755 | 38.174 | 55.348 | 36.931 | 1.00 | 0.00 |
| ATOM | 2460 H | ARG | S | 755 | 34.954 | 58.860 | 34.414 | 1.00 | 0.00 |
| ATOM | 2461 HE | ARG | S | 755 | 36.081 | 53.010 | 36.212 | 1.00 | 0.00 |
| ATOM | 2462 1HH1 | ARG | S | 755 | 39.248 | 53.208 | 37.664 | 1.00 | 0.00 |
| ATOM | 2463 2HH1 | ARG | S | 755 | 37.968 | 52.156 | 37.330 | 1.00 | 0.00 |
| ATOM | 2464 1HH2 | ARG | S | 755 | 39.105 | 55.457 | 37.299 | 1.00 | 0.00 |
| ATOM | 2465 2HH2 | ARG | S | 755 | 37.674 | 56.159 | 36.621 | 1.00 | 0.00 |
| ATOM | 2466 N | SER | S | 756 | 37.700 | 58.140 | 31.559 | 1.00 | 0.00 |
| ATOM | 2467 CA | SER | S | 756 | 37.931 | 59.358 | 30.777 | 1.00 | 0.00 |
| ATOM | 2468 C | SER | S | 756 | 37.310 | 59.492 | 29.394 | 1.00 | 0.00 |
| ATOM | 2469 O | SER | S | 756 | 37.343 | 58.578 | 28.572 | 1.00 | 0.00 |
| ATOM | 2470 CB | SER | S | 756 | 39.434 | 59.612 | 30.748 | 1.00 | 0.00 |
| ATOM | 2471 OG | SER | S | 756 | 39.994 | 59.112 | 31.982 | 1.00 | 0.00 |
| ATOM | 2472 H | SER | S | 756 | 38.409 | 57.785 | 32.169 | 1.00 | 0.00 |
| ATOM | 2473 HG | SER | S | 756 | 39.389 | 59.351 | 32.693 | 1.00 | 0.00 |
| ATOM | 2474 N | GLY | S | 757 | 36.791 | 60.707 | 29.134 | 1.00 | 0.00 |
| ATOM | 2475 CA | GLY | S | 757 | 36.362 | 61.073 | 27.778 | 1.00 | 0.00 |
| ATOM | 2476 C | GLY | S | 757 | 35.402 | 60.114 | 27.087 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2477 O | GLY | S | 757 | 34.470 | 59.570 | 27.684 | 1.00 | 0.00 |
| ATOM | 2478 H | GLY | S | 757 | 36.746 | 61.373 | 29.885 | 1.00 | 0.00 |
| ATOM | 2479 N | PHE | S | 758 | 35.699 | 59.921 | 25.797 | 1.00 | 0.00 |
| ATOM | 2480 CA | PHE | S | 758 | 35.162 | 58.836 | 24.976 | 1.00 | 0.00 |
| ATOM | 2481 C | PHE | S | 758 | 36.245 | 58.413 | 24.004 | 1.00 | 0.00 |
| ATOM | 2482 O | PHE | S | 758 | 36.755 | 59.218 | 23.222 | 1.00 | 0.00 |
| ATOM | 2483 CB | PHE | S | 758 | 33.917 | 59.260 | 24.184 | 1.00 | 0.00 |
| ATOM | 2484 CG | PHE | S | 758 | 32.719 | 59.440 | 25.088 | 1.00 | 0.00 |
| ATOM | 2485 CD1 | PHE | S | 758 | 32.104 | 58.305 | 25.663 | 1.00 | 0.00 |
| ATOM | 2486 CD2 | PHE | S | 758 | 32.233 | 60.741 | 25.339 | 1.00 | 0.00 |
| ATOM | 2487 CE1 | PHE | S | 758 | 30.991 | 58.474 | 26.507 | 1.00 | 0.00 |
| ATOM | 2488 CE2 | PHE | S | 758 | 31.118 | 60.912 | 26.183 | 1.00 | 0.00 |
| ATOM | 2489 CZ | PHE | S | 758 | 30.511 | 59.776 | 26.760 | 1.00 | 0.00 |
| ATOM | 2490 H | PHE | S | 758 | 36.369 | 60.512 | 25.343 | 1.00 | 0.00 |
| ATOM | 2491 N | GLY | S | 759 | 36.632 | 57.123 | 24.086 | 1.00 | 0.00 |
| ATOM | 2492 CA | GLY | S | 759 | 37.848 | 56.759 | 23.344 | 1.00 | 0.00 |
| ATOM | 2493 C | GLY | S | 759 | 37.819 | 55.454 | 22.561 | 1.00 | 0.00 |
| ATOM | 2494 O | GLY | S | 759 | 37.263 | 54.455 | 23.004 | 1.00 | 0.00 |
| ATOM | 2495 H | GLY | S | 759 | 36.167 | 56.514 | 24.727 | 1.00 | 0.00 |
| ATOM | 2496 N | ILE | S | 760 | 38.454 | 55.520 | 21.368 | 1.00 | 0.00 |
| ATOM | 2497 CA | ILE | S | 760 | 38.690 | 54.387 | 20.447 | 1.00 | 0.00 |
| ATOM | 2498 C | ILE | S | 760 | 39.931 | 53.621 | 20.906 | 1.00 | 0.00 |
| ATOM | 2499 O | ILE | S | 760 | 40.691 | 54.186 | 21.678 | 1.00 | 0.00 |
| ATOM | 2500 CB | ILE | S | 760 | 38.893 | 54.952 | 19.016 | 1.00 | 0.00 |
| ATOM | 2501 CG1 | ILE | S | 760 | 39.051 | 53.901 | 17.914 | 1.00 | 0.00 |
| ATOM | 2502 CG2 | ILE | S | 760 | 40.101 | 55.889 | 18.959 | 1.00 | 0.00 |
| ATOM | 2503 CD1 | ILE | S | 760 | 39.332 | 54.482 | 16.527 | 1.00 | 0.00 |
| ATOM | 2504 H | ILE | S | 760 | 38.926 | 56.386 | 21.211 | 1.00 | 0.00 |
| ATOM | 2505 N | GLY | S | 761 | 40.151 | 52.381 | 20.440 | 1.00 | 0.00 |
| ATOM | 2506 CA | GLY | S | 761 | 41.475 | 51.816 | 20.740 | 1.00 | 0.00 |
| ATOM | 2507 C | GLY | S | 761 | 41.588 | 50.302 | 20.671 | 1.00 | 0.00 |
| ATOM | 2508 O | GLY | S | 761 | 40.758 | 49.558 | 21.189 | 1.00 | 0.00 |
| ATOM | 2509 H | GLY | S | 761 | 39.492 | 51.886 | 19.866 | 1.00 | 0.00 |
| ATOM | 2510 N | MET | S | 762 | 42.647 | 49.858 | 19.987 | 1.00 | 0.00 |
| ATOM | 2511 CA | MET | S | 762 | 42.815 | 48.433 | 19.682 | 1.00 | 0.00 |
| ATOM | 2512 C | MET | S | 762 | 43.591 | 47.585 | 20.685 | 1.00 | 0.00 |
| ATOM | 2513 O | MET | S | 762 | 44.808 | 47.439 | 20.601 | 1.00 | 0.00 |
| ATOM | 2514 CB | MET | S | 762 | 43.424 | 48.314 | 18.276 | 1.00 | 0.00 |
| ATOM | 2515 CG | MET | S | 762 | 43.706 | 46.897 | 17.767 | 1.00 | 0.00 |
| ATOM | 2516 SD | MET | S | 762 | 44.297 | 46.876 | 16.072 | 1.00 | 0.00 |
| ATOM | 2517 CE | MET | S | 762 | 44.615 | 45.110 | 15.939 | 1.00 | 0.00 |
| ATOM | 2518 H | MET | S | 762 | 43.303 | 50.556 | 19.701 | 1.00 | 0.00 |
| ATOM | 2519 N | ARG | S | 763 | 42.836 | 46.950 | 21.594 | 1.00 | 0.00 |
| ATOM | 2520 CA | ARG | S | 763 | 43.374 | 45.926 | 22.506 | 1.00 | 0.00 |
| ATOM | 2521 C | ARG | S | 763 | 44.472 | 46.443 | 23.443 | 1.00 | 0.00 |
| ATOM | 2522 O | ARG | S | 763 | 44.373 | 47.646 | 23.672 | 1.00 | 0.00 |
| ATOM | 2523 CB | ARG | S | 763 | 43.798 | 44.675 | 21.709 | 1.00 | 0.00 |
| ATOM | 2524 CG | ARG | S | 763 | 43.324 | 43.362 | 22.330 | 1.00 | 0.00 |
| ATOM | 2525 CD | ARG | S | 763 | 44.026 | 42.090 | 21.812 | 1.00 | 0.00 |
| ATOM | 2526 NE | ARG | S | 763 | 44.037 | 41.910 | 20.353 | 1.00 | 0.00 |
| ATOM | 2527 CZ | ARG | S | 763 | 42.925 | 41.707 | 19.598 | 1.00 | 0.00 |
| ATOM | 2528 NH1 | ARG | S | 763 | 41.708 | 41.767 | 20.124 | 1.00 | 0.00 |
| ATOM | 2529 NH2 | ARG | S | 763 | 43.054 | 41.455 | 18.301 | 1.00 | 0.00 |
| ATOM | 2530 H | ARG | S | 763 | 41.855 | 47.080 | 21.469 | 1.00 | 0.00 |
| ATOM | 2531 HE | ARG | S | 763 | 44.972 | 41.889 | 19.917 | 1.00 | 0.00 |
| ATOM | 2532 1HH1 | ARG | S | 763 | 40.867 | 41.715 | 19.576 | 1.00 | 0.00 |
| ATOM | 2533 2HH1 | ARG | S | 763 | 41.593 | 41.859 | 21.116 | 1.00 | 0.00 |
| ATOM | 2534 1HH2 | ARG | S | 763 | 42.263 | 41.528 | 17.681 | 1.00 | 0.00 |
| ATOM | 2535 2HH2 | ARG | S | 763 | 43.927 | 41.204 | 17.880 | 1.00 | 0.00 |
| ATOM | 2536 N | LYS | S | 764 | 45.289 | 45.526 | 23.983 | 1.00 | 0.00 |
| ATOM | 2537 CA | LYS | S | 764 | 46.654 | 45.953 | 24.286 | 1.00 | 0.00 |
| ATOM | 2538 C | LYS | S | 764 | 47.540 | 45.593 | 23.105 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2539 O | LYS | S | 764 | 48.636 | 45.048 | 23.214 | 1.00 | 0.00 |
| ATOM | 2540 CB | LYS | S | 764 | 47.183 | 45.292 | 25.564 | 1.00 | 0.00 |
| ATOM | 2541 CG | LYS | S | 764 | 48.079 | 46.194 | 26.428 | 1.00 | 0.00 |
| ATOM | 2542 CD | LYS | S | 764 | 47.242 | 47.252 | 27.147 | 1.00 | 0.00 |
| ATOM | 2543 CE | LYS | S | 764 | 47.946 | 48.166 | 28.153 | 1.00 | 0.00 |
| ATOM | 2544 NZ | LYS | S | 764 | 46.892 | 48.864 | 28.886 | 1.00 | 0.00 |
| ATOM | 2545 H | LYS | S | 764 | 45.095 | 44.549 | 23.913 | 1.00 | 0.00 |
| ATOM | 2546 1HZ | LYS | S | 764 | 46.079 | 49.138 | 28.306 | 1.00 | 0.00 |
| ATOM | 2547 2HZ | LYS | S | 764 | 47.204 | 49.705 | 29.407 | 1.00 | 0.00 |
| ATOM | 2548 3HZ | LYS | S | 764 | 46.510 | 48.238 | 29.612 | 1.00 | 0.00 |
| ATOM | 2549 N | ASP | S | 765 | 46.986 | 45.860 | 21.907 | 1.00 | 0.00 |
| ATOM | 2550 CA | ASP | S | 765 | 47.820 | 45.464 | 20.780 | 1.00 | 0.00 |
| ATOM | 2551 C | ASP | S | 765 | 48.819 | 46.569 | 20.561 | 1.00 | 0.00 |
| ATOM | 2552 O | ASP | S | 765 | 48.791 | 47.602 | 21.235 | 1.00 | 0.00 |
| ATOM | 2553 CB | ASP | S | 765 | 47.003 | 45.101 | 19.528 | 1.00 | 0.00 |
| ATOM | 2554 CG | ASP | S | 765 | 47.728 | 44.023 | 18.727 | 1.00 | 0.00 |
| ATOM | 2555 OD1 | ASP | S | 765 | 47.448 | 42.839 | 18.920 | 1.00 | 0.00 |
| ATOM | 2556 OD2 | ASP | S | 765 | 48.583 | 44.359 | 17.909 | 1.00 | 0.00 |
| ATOM | 2557 H | ASP | S | 765 | 46.272 | 46.553 | 21.783 | 1.00 | 0.00 |
| ATOM | 2558 N | SER | S | 766 | 49.741 | 46.304 | 19.661 | 1.00 | 0.00 |
| ATOM | 2559 CA | SER | S | 766 | 50.706 | 47.356 | 19.453 | 1.00 | 0.00 |
| ATOM | 2560 C | SER | S | 766 | 50.868 | 47.795 | 18.012 | 1.00 | 0.00 |
| ATOM | 2561 O | SER | S | 766 | 50.593 | 48.956 | 17.731 | 1.00 | 0.00 |
| ATOM | 2562 CB | SER | S | 766 | 51.992 | 47.073 | 20.238 | 1.00 | 0.00 |
| ATOM | 2563 OG | SER | S | 766 | 52.307 | 45.674 | 20.160 | 1.00 | 0.00 |
| ATOM | 2564 H | SER | S | 766 | 49.713 | 45.456 | 19.134 | 1.00 | 0.00 |
| ATOM | 2565 HG | SER | S | 766 | 51.756 | 45.255 | 20.824 | 1.00 | 0.00 |
| ATOM | 2566 N | PRO | S | 767 | 51.280 | 46.898 | 17.065 | 1.00 | 0.00 |
| ATOM | 2567 CA | PRO | S | 767 | 51.536 | 47.418 | 15.720 | 1.00 | 0.00 |
| ATOM | 2568 C | PRO | S | 767 | 50.315 | 47.959 | 14.987 | 1.00 | 0.00 |
| ATOM | 2569 O | PRO | S | 767 | 50.463 | 48.601 | 13.951 | 1.00 | 0.00 |
| ATOM | 2570 CB | PRO | S | 767 | 52.197 | 46.232 | 15.010 | 1.00 | 0.00 |
| ATOM | 2571 CG | PRO | S | 767 | 51.622 | 44.998 | 15.697 | 1.00 | 0.00 |
| ATOM | 2572 CD | PRO | S | 767 | 51.527 | 45.457 | 17.145 | 1.00 | 0.00 |
| ATOM | 2573 N | TRP | S | 768 | 49.127 | 47.687 | 15.545 | 1.00 | 0.00 |
| ATOM | 2574 CA | TRP | S | 768 | 48.009 | 48.426 | 14.989 | 1.00 | 0.00 |
| ATOM | 2575 C | TRP | S | 768 | 47.272 | 49.326 | 15.957 | 1.00 | 0.00 |
| ATOM | 2576 O | TRP | S | 768 | 46.673 | 50.315 | 15.550 | 1.00 | 0.00 |
| ATOM | 2577 CB | TRP | S | 768 | 47.075 | 47.528 | 14.192 | 1.00 | 0.00 |
| ATOM | 2578 CG | TRP | S | 768 | 46.448 | 48.338 | 13.081 | 1.00 | 0.00 |
| ATOM | 2579 CD1 | TRP | S | 768 | 45.101 | 48.711 | 12.974 | 1.00 | 0.00 |
| ATOM | 2580 CD2 | TRP | S | 768 | 47.080 | 48.853 | 11.887 | 1.00 | 0.00 |
| ATOM | 2581 NE1 | TRP | S | 768 | 44.871 | 49.393 | 11.820 | 1.00 | 0.00 |
| ATOM | 2582 CE2 | TRP | S | 768 | 46.062 | 49.507 | 11.116 | 1.00 | 0.00 |
| ATOM | 2583 CE3 | TRP | S | 768 | 48.405 | 48.805 | 11.400 | 1.00 | 0.00 |
| ATOM | 2584 CZ2 | TRP | S | 768 | 46.385 | 50.192 | 9.873 | 1.00 | 0.00 |
| ATOM | 2585 CZ3 | TRP | S | 768 | 48.716 | 49.396 | 10.157 | 1.00 | 0.00 |
| ATOM | 2586 CH2 | TRP | S | 768 | 47.711 | 50.034 | 9.397 | 1.00 | 0.00 |
| ATOM | 2587 H | TRP | S | 768 | 49.000 | 47.028 | 16.284 | 1.00 | 0.00 |
| ATOM | 2588 HE1 | TRP | S | 768 | 43.990 | 49.652 | 11.466 | 1.00 | 0.00 |
| ATOM | 2589 N | LYS | S | 769 | 47.392 | 49.035 | 17.260 | 1.00 | 0.00 |
| ATOM | 2590 CA | LYS | S | 769 | 47.031 | 50.104 | 18.203 | 1.00 | 0.00 |
| ATOM | 2591 C | LYS | S | 769 | 47.843 | 51.385 | 18.018 | 1.00 | 0.00 |
| ATOM | 2592 O | LYS | S | 769 | 47.432 | 52.497 | 18.338 | 1.00 | 0.00 |
| ATOM | 2593 CB | LYS | S | 769 | 47.114 | 49.581 | 19.637 | 1.00 | 0.00 |
| ATOM | 2594 CG | LYS | S | 769 | 46.207 | 50.243 | 20.683 | 1.00 | 0.00 |
| ATOM | 2595 CD | LYS | S | 769 | 46.667 | 51.592 | 21.223 | 1.00 | 0.00 |
| ATOM | 2596 CE | LYS | S | 769 | 45.581 | 52.249 | 22.068 | 1.00 | 0.00 |
| ATOM | 2597 NZ | LYS | S | 769 | 46.014 | 53.591 | 22.444 | 1.00 | 0.00 |
| ATOM | 2598 H | LYS | S | 769 | 47.753 | 48.159 | 17.577 | 1.00 | 0.00 |
| ATOM | 2599 1HZ | LYS | S | 769 | 45.134 | 54.112 | 22.605 | 1.00 | 0.00 |
| ATOM | 2600 2HZ | LYS | S | 769 | 46.567 | 54.025 | 21.675 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2601 3HZ | LYS | S | 769 | 46.526 | 53.550 | 23.349 | 1.00 | 0.00 |
| ATOM | 2602 N | GLN | S | 770 | 49.034 | 51.183 | 17426 | 1.00 | 0.00 |
| ATOM | 2603 CA | GLN | S | 770 | 49.857 | 52.269 | 16.894 | 1.00 | 0.00 |
| ATOM | 2604 C | GLN | S | 770 | 49.097 | 53.119 | 15.896 | 1.00 | 0.00 |
| ATOM | 2605 O | GLN | S | 770 | 48.855 | 54.305 | 16.120 | 1.00 | 0.00 |
| ATOM | 2606 CB | GLN | S | 770 | 51.142 | 51.649 | 16.324 | 1.00 | 0.00 |
| ATOM | 2607 CG | GLN | S | 770 | 52.089 | 52.518 | 15.492 | 1.00 | 0.00 |
| ATOM | 2608 CD | GLN | S | 770 | 51.843 | 52.352 | 13.998 | 1.00 | 0.00 |
| ATOM | 2609 OE1 | GLN | S | 770 | 51.855 | 53.307 | 13.230 | 1.00 | 0.00 |
| ATOM | 2610 NE2 | GLN | S | 770 | 51.741 | 51.095 | 13.557 | 1.00 | 0.00 |
| ATOM | 2611 H | GLN | S | 770 | 49.297 | 50.231 | 17.295 | 1.00 | 0.00 |
| ATOM | 2612 1HE2 | GLN | S | 770 | 51.962 | 50.904 | 12.601 | 1.00 | 0.00 |
| ATOM | 2613 2HE2 | GLN | S | 770 | 51.442 | 50.347 | 14.152 | 1.00 | 0.00 |
| ATOM | 2614 N | ASN | S | 771 | 48.663 | 52.427 | 14.819 | 1.00 | 0.00 |
| ATOM | 2615 CA | ASN | S | 771 | 47.900 | 53.177 | 13.820 | 1.00 | 0.00 |
| ATOM | 2616 C | ASN | S | 771 | 46.658 | 53.841 | 14.352 | 1.00 | 0.00 |
| ATOM | 2617 O | ASN | S | 771 | 46.340 | 54.964 | 14.000 | 1.00 | 0.00 |
| ATOM | 2618 CB | ASN | S | 771 | 47.517 | 52.369 | 12.590 | 1.00 | 0.00 |
| ATOM | 2619 CG | ASN | S | 771 | 47.271 | 53.337 | 11.445 | 1.00 | 0.00 |
| ATOM | 2620 OD1 | ASN | S | 771 | 46.168 | 53.729 | 11.077 | 1.00 | 0.00 |
| ATOM | 2621 ND2 | ASN | S | 771 | 48.406 | 53.701 | 10.843 | 1.00 | 0.00 |
| ATOM | 2622 H | ASN | S | 771 | 48.910 | 51.473 | 14.669 | 1.00 | 0.00 |
| ATOM | 2623 1HD2 | ASN | S | 771 | 48.347 | 54.228 | 9.994 | 1.00 | 0.00 |
| ATOM | 2624 2HD2 | ASN | S | 771 | 49.301 | 53.497 | 11.237 | 1.00 | 0.00 |
| ATOM | 2625 N | VAL | S | 772 | 46.001 | 53.150 | 15.286 | 1.00 | 0.00 |
| ATOM | 2626 CA | VAL | S | 772 | 44.888 | 53.802 | 15.991 | 1.00 | 0.00 |
| ATOM | 2627 C | VAL | S | 772 | 45.276 | 55.056 | 16.775 | 1.00 | 0.00 |
| ATOM | 2628 O | VAL | S | 772 | 44.606 | 56.089 | 16.806 | 1.00 | 0.00 |
| ATOM | 2629 CB | VAL | S | 772 | 44.200 | 52.772 | 16.890 | 1.00 | 0.00 |
| ATOM | 2630 CG1 | VAL | S | 772 | 42.996 | 53.345 | 17.639 | 1.00 | 0.00 |
| ATOM | 2631 CG2 | VAL | S | 772 | 43.823 | 51.553 | 16.052 | 1.00 | 0.00 |
| ATOM | 2632 H | VAL | S | 772 | 46.389 | 52.258 | 15.526 | 1.00 | 0.00 |
| ATOM | 2633 N | SER | S | 773 | 46.443 | 54.956 | 17.410 | 1.00 | 0.00 |
| ATOM | 2634 CA | SER | S | 773 | 46.924 | 56.157 | 18.085 | 1.00 | 0.00 |
| ATOM | 2635 C | SER | S | 773 | 47.550 | 57.192 | 17.134 | 1.00 | 0.00 |
| ATOM | 2636 O | SER | S | 773 | 47.718 | 58.369 | 17.430 | 1.00 | 0.00 |
| ATOM | 2637 CB | SER | S | 773 | 47.783 | 55.736 | 19.290 | 1.00 | 0.00 |
| ATOM | 2638 OG | SER | S | 773 | 47.076 | 54.744 | 20.079 | 1.00 | 0.00 |
| ATOM | 2639 H | SER | S | 773 | 46.987 | 54.123 | 17.325 | 1.00 | 0.00 |
| ATOM | 2640 HG | SER | S | 773 | 46.839 | 54.078 | 19.430 | 1.00 | 0.00 |
| ATOM | 2641 N | LEU | S | 774 | 47.822 | 56.730 | 15.902 | 1.00 | 0.00 |
| ATOM | 2642 CA | LEU | S | 774 | 48.089 | 57.690 | 14.831 | 1.00 | 0.00 |
| ATOM | 2643 C | LEU | S | 774 | 46.803 | 58.327 | 14.323 | 1.00 | 0.00 |
| ATOM | 2644 O | LEU | S | 774 | 46.720 | 59.513 | 14.011 | 1.00 | 0.00 |
| ATOM | 2645 CB | LEU | S | 774 | 48.872 | 57.005 | 13.705 | 1.00 | 0.00 |
| ATOM | 2646 CG | LEU | S | 774 | 49.319 | 57.929 | 12.569 | 1.00 | 0.00 |
| ATOM | 2647 CD1 | LEU | S | 774 | 50.255 | 59.038 | 13.055 | 1.00 | 0.00 |
| ATOM | 2648 CD2 | LEU | S | 774 | 49.921 | 57.134 | 11.410 | 1.00 | 0.00 |
| ATOM | 2649 H | LEU | S | 774 | 47.656 | 55.764 | 15.714 | 1.00 | 0.00 |
| ATOM | 2650 N | SER | S | 775 | 45.762 | 57.489 | 14.303 | 1.00 | 0.00 |
| ATOM | 2651 CA | SER | S | 775 | 44.429 | 57.965 | 13.944 | 1.00 | 0.00 |
| ATOM | 2652 C | SER | S | 775 | 43.928 | 59.041 | 14.892 | 1.00 | 0.00 |
| ATOM | 2653 O | SER | S | 775 | 43.333 | 60.048 | 14.509 | 1.00 | 0.00 |
| ATOM | 2654 CB | SER | S | 775 | 43.467 | 56.780 | 13.801 | 1.00 | 0.00 |
| ATOM | 2655 OG | SER | S | 775 | 43.971 | 55.841 | 12.829 | 1.00 | 0.00 |
| ATOM | 2656 H | SER | S | 775 | 45.819 | 56.595 | 14.737 | 1.00 | 0.00 |
| ATOM | 2657 HG | SER | S | 775 | 44.802 | 55.543 | 13.192 | 1.00 | 0.00 |
| ATOM | 2658 N | ILE | S | 776 | 44.346 | 58.887 | 16.152 | 1.00 | 0.00 |
| ATOM | 2659 CA | ILE | S | 776 | 44.151 | 59.964 | 17.120 | 1.00 | 0.00 |
| ATOM | 2660 C | ILE | S | 776 | 44.585 | 61.386 | 16.743 | 1.00 | 0.00 |
| ATOM | 2661 O | ILE | S | 776 | 44.103 | 62.383 | 17.278 | 1.00 | 0.00 |
| ATOM | 2662 CB | ILE | S | 776 | 44.623 | 59.480 | 18.500 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2663 CG1 | ILE | S | 776 | 43.434 | 59.556 | 19.446 | 1.00 | 0.00 |
| ATOM | 2664 CG2 | ILE | S | 776 | 45.835 | 60.234 | 19.066 | 1.00 | 0.00 |
| ATOM | 2665 CD1 | ILE | S | 776 | 42.199 | 58.898 | 18.833 | 1.00 | 0.00 |
| ATOM | 2666 H | ILE | S | 776 | 44.675 | 57.982 | 16.396 | 1.00 | 0.00 |
| ATOM | 2667 N | LEU | S | 777 | 45.473 | 61.437 | 15.737 | 1.00 | 0.00 |
| ATOM | 2668 CA | LEU | S | 777 | 45.677 | 62.706 | 15.030 | 1.00 | 0.00 |
| ATOM | 2669 C | LEU | S | 777 | 44.951 | 62.804 | 13.683 | 1.00 | 0.00 |
| ATOM | 2670 O | LEU | S | 777 | 44.404 | 63.832 | 13.291 | 1.00 | 0.00 |
| ATOM | 2671 CB | LEU | S | 777 | 47.197 | 62.958 | 14.866 | 1.00 | 0.00 |
| ATOM | 2672 CG | LEU | S | 777 | 47.537 | 64.361 | 14.364 | 1.00 | 0.00 |
| ATOM | 2673 CD1 | LEU | S | 777 | 47.069 | 65.456 | 15.325 | 1.00 | 0.00 |
| ATOM | 2674 CD2 | LEU | S | 777 | 49.027 | 64.479 | 14.043 | 1.00 | 0.00 |
| ATOM | 2675 H | LEU | S | 777 | 45.867 | 60.564 | 15.458 | 1.00 | 0.00 |
| ATOM | 2676 N | LYS | S | 778 | 44.980 | 61.665 | 12.959 | 1.00 | 0.00 |
| ATOM | 2677 CA | LYS | S | 778 | 44.311 | 61.538 | 11.648 | 1.00 | 0.00 |
| ATOM | 2678 C | LYS | S | 778 | 42.822 | 61.931 | 11.599 | 1.00 | 0.00 |
| ATOM | 2679 O | LYS | S | 778 | 42.207 | 63.170 | 10.557 | 1.00 | 0.00 |
| ATOM | 2680 CB | LYS | S | 778 | 44.582 | 60.113 | 11.132 | 1.00 | 0.00 |
| ATOM | 2681 CG | LYS | S | 778 | 43.952 | 59.707 | 9.798 | 1.00 | 0.00 |
| ATOM | 2682 CD | LYS | S | 778 | 44.444 | 60.538 | 8.616 | 1.00 | 0.00 |
| ATOM | 2683 CE | LYS | S | 778 | 43.404 | 60.586 | 7.496 | 1.00 | 0.00 |
| ATOM | 2684 NZ | LYS | S | 778 | 42.190 | 61.231 | 8.018 | 1.00 | 0.00 |
| ATOM | 2685 H | LYS | S | 778 | 45.416 | 60.866 | 13.363 | 1.00 | 0.00 |
| ATOM | 2686 1HZ | LYS | S | 778 | 41.756 | 61.885 | 7.328 | 1.00 | 0.00 |
| ATOM | 2687 2HZ | LYS | S | 778 | 41.509 | 60.496 | 8.287 | 1.00 | 0.00 |
| ATOM | 2688 3HZ | LYS | S | 778 | 42.423 | 61.779 | 8.870 | 1.00 | 0.00 |
| ATOM | 2689 N | SER | S | 779 | 42.255 | 62.061 | 12.805 | 1.00 | 0.00 |
| ATOM | 2690 CA | SER | S | 779 | 41.015 | 62.801 | 12.996 | 1.00 | 0.00 |
| ATOM | 2691 C | SER | S | 779 | 41.048 | 64.213 | 12.406 | 1.00 | 0.00 |
| ATOM | 2692 O | SER | S | 779 | 40.323 | 64.499 | 11.457 | 1.00 | 0.00 |
| ATOM | 2693 CB | SER | S | 779 | 40.665 | 62.743 | 14.489 | 1.00 | 0.00 |
| ATOM | 2694 OG | SER | S | 779 | 40.696 | 61.362 | 14.909 | 1.00 | 0.00 |
| ATOM | 2695 H | SER | S | 779 | 42.741 | 61.706 | 13.601 | 1.00 | 0.00 |
| ATOM | 2696 HG | SER | S | 779 | 40.118 | 60.927 | 14.277 | 1.00 | 0.00 |
| ATOM | 2697 N | HIS | S | 780 | 41.940 | 65.059 | 12.947 | 1.00 | 0.00 |
| ATOM | 2698 CA | HIS | S | 780 | 42.063 | 66.406 | 12.385 | 1.00 | 0.00 |
| ATOM | 2699 C | HIS | S | 780 | 42.461 | 66.378 | 10.917 | 1.00 | 0.00 |
| ATOM | 2700 O | HIS | S | 780 | 41.742 | 66.857 | 10.039 | 1.00 | 0.00 |
| ATOM | 2701 CB | HIS | S | 780 | 43.066 | 67.258 | 13.178 | 1.00 | 0.00 |
| ATOM | 2702 CG | HIS | S | 780 | 42.711 | 67.376 | 14.646 | 1.00 | 0.00 |
| ATOM | 2703 ND1 | HIS | S | 780 | 41.496 | 67.708 | 15.116 | 1.00 | 0.00 |
| ATOM | 2704 CD2 | HIS | S | 780 | 43.570 | 67.199 | 15.738 | 1.00 | 0.00 |
| ATOM | 2705 CE1 | HIS | S | 780 | 41.578 | 67.743 | 16.481 | 1.00 | 0.00 |
| ATOM | 2706 NE2 | HIS | S | 780 | 42.859 | 67.432 | 16.871 | 1.00 | 0.00 |
| ATOM | 2707 H | HIS | S | 780 | 42.514 | 64.769 | 13.713 | 1.00 | 0.00 |
| ATOM | 2708 HD1 | HIS | S | 780 | 40.689 | 67.917 | 14.596 | 1.00 | 0.00 |
| ATOM | 2709 N | GLU | S | 781 | 43.645 | 65.752 | 10.707 | 1.00 | 0.00 |
| ATOM | 2710 CA | GLU | S | 781 | 44.211 | 65.523 | 9.370 | 1.00 | 0.00 |
| ATOM | 2711 C | GLU | S | 781 | 44.538 | 66.778 | 8.558 | 1.00 | 0.00 |
| ATOM | 2712 O | GLU | S | 781 | 45.686 | 67.182 | 8.393 | 1.00 | 0.00 |
| ATOM | 2713 CB | GLU | S | 781 | 43.308 | 64.539 | 8.617 | 1.00 | 0.00 |
| ATOM | 2714 CG | GLU | S | 781 | 43.651 | 64.249 | 7.158 | 1.00 | 0.00 |
| ATOM | 2715 CD | GLU | S | 781 | 42.332 | 64.169 | 6.422 | 1.00 | 0.00 |
| ATOM | 2716 OE1 | GLU | S | 781 | 41.920 | 63.079 | 6.037 | 1.00 | 0.00 |
| ATOM | 2717 OE2 | GLU | S | 781 | 41.703 | 65.208 | 6.253 | 1.00 | 0.00 |
| ATOM | 2718 H | GLU | S | 781 | 44.180 | 65.466 | 11.501 | 1.00 | 0.00 |
| ATOM | 2719 N | ASN | S | 782 | 43.465 | 67.387 | 8.033 | 1.00 | 0.00 |
| ATOM | 2720 CA | ASN | S | 782 | 43.553 | 68.648 | 7.298 | 1.00 | 0.00 |
| ATOM | 2721 C | ASN | S | 782 | 42.766 | 69.715 | 8.032 | 1.00 | 0.00 |
| ATOM | 2722 O | ASN | S | 782 | 42.049 | 70.537 | 7.465 | 1.00 | 0.00 |
| ATOM | 2723 CB | ASN | S | 782 | 43.005 | 68.481 | 5.881 | 1.00 | 0.00 |
| ATOM | 2724 CG | ASN | S | 782 | 44.107 | 68.041 | 4.943 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2725 OD1 | ASN | S | 782 | 44.940 | 68.828 | 4.503 | 1.00 | 0.00 |
| ATOM | 2726 ND2 | ASN | S | 782 | 44.067 | 66.748 | 4.604 | 1.00 | 0.00 |
| ATOM | 2727 H | ASN | S | 782 | 42.565 | 67.024 | 8.273 | 1.00 | 0.00 |
| ATOM | 2728 1HD2 | ASN | S | 782 | 44.734 | 66.400 | 3.950 | 1.00 | 0.00 |
| ATOM | 2729 2HD2 | ASN | S | 782 | 43.373 | 66.138 | 5.002 | 1.00 | 0.00 |
| ATOM | 2730 N | GLY | S | 783 | 42.899 | 69.632 | 9.363 | 1.00 | 0.00 |
| ATOM | 2731 CA | GLY | S | 783 | 42.081 | 70.480 | 10.228 | 1.00 | 0.00 |
| ATOM | 2732 C | GLY | S | 783 | 40.659 | 69.971 | 10.406 | 1.00 | 0.00 |
| ATOM | 2733 O | GLY | S | 783 | 40.272 | 69.473 | 11.464 | 1.00 | 0.00 |
| ATOM | 2734 H | GLY | S | 783 | 43.432 | 68.879 | 9.740 | 1.00 | 0.00 |
| ATOM | 2735 N | PHE | S | 784 | 39.908 | 70.145 | 9.302 | 1.00 | 0.00 |
| ATOM | 2736 CA | PHE | S | 784 | 38.464 | 69.933 | 9.278 | 1.00 | 0.00 |
| ATOM | 2737 C | PHE | S | 784 | 37.983 | 68.739 | 10.075 | 1.00 | 0.00 |
| ATOM | 2738 O | PHE | S | 784 | 38.308 | 67.586 | 9.792 | 1.00 | 0.00 |
| ATOM | 2739 CB | PHE | S | 784 | 37.977 | 69.870 | 7.826 | 1.00 | 0.00 |
| ATOM | 2740 CG | PHE | S | 784 | 36.477 | 70.054 | 7.748 | 1.00 | 0.00 |
| ATOM | 2741 CD1 | PHE | S | 784 | 35.923 | 71.336 | 7.956 | 1.00 | 0.00 |
| ATOM | 2742 CD2 | PHE | S | 784 | 35.656 | 68.941 | 7.462 | 1.00 | 0.00 |
| ATOM | 2743 CE1 | PHE | S | 784 | 34.527 | 71.510 | 7.873 | 1.00 | 0.00 |
| ATOM | 2744 CE2 | PHE | S | 784 | 34.261 | 69.115 | 7.378 | 1.00 | 0.00 |
| ATOM | 2745 CZ | PHE | S | 784 | 33.711 | 70.396 | 7.584 | 1.00 | 0.00 |
| ATOM | 2746 H | PHE | S | 784 | 40.379 | 70.456 | 8.481 | 1.00 | 0.00 |
| ATOM | 2747 N | MET | S | 785 | 37.212 | 69.105 | 11.111 | 1.00 | 0.00 |
| ATOM | 2748 CA | MET | S | 785 | 36.642 | 68.115 | 12.026 | 1.00 | 0.00 |
| ATOM | 2749 C | MET | S | 785 | 35.302 | 68.609 | 12.558 | 1.00 | 0.00 |
| ATOM | 2750 O | MET | S | 785 | 35.103 | 68.857 | 13.746 | 1.00 | 0.00 |
| ATOM | 2751 CB | MET | S | 785 | 37.650 | 67.834 | 13.150 | 1.00 | 0.00 |
| ATOM | 2752 CG | MET | S | 785 | 37.451 | 66.516 | 13.903 | 1.00 | 0.00 |
| ATOM | 2753 SD | MET | S | 785 | 38.604 | 66.355 | 15.281 | 1.00 | 0.00 |
| ATOM | 2754 CE | MET | S | 785 | 37.964 | 64.827 | 15.980 | 1.00 | 0.00 |
| ATOM | 2755 H | MET | S | 785 | 37.090 | 70.085 | 11.288 | 1.00 | 0.00 |
| ATOM | 2756 N | GLU | S | 786 | 34.409 | 68.834 | 11.587 | 1.00 | 0.00 |
| ATOM | 2757 CA | GLU | S | 786 | 33.137 | 69.433 | 11.971 | 1.00 | 0.00 |
| ATOM | 2758 C | GLU | S | 786 | 31.971 | 68.504 | 11.725 | 1.00 | 0.00 |
| ATOM | 2759 O | GLU | S | 786 | 31.189 | 68.176 | 12.611 | 1.00 | 0.00 |
| ATOM | 2760 CB | GLU | S | 786 | 32.958 | 70.798 | 11.292 | 1.00 | 0.00 |
| ATOM | 2761 CG | GLU | S | 786 | 33.873 | 71.904 | 11.858 | 1.00 | 0.00 |
| ATOM | 2762 CD | GLU | S | 786 | 33.522 | 72.256 | 13.302 | 1.00 | 0.00 |
| ATOM | 2763 OE1 | GLU | S | 786 | 32.508 | 71.792 | 13.810 | 1.00 | 0.00 |
| ATOM | 2764 OE2 | GLU | S | 786 | 34.256 | 72.999 | 13.851 | 1.00 | 0.00 |
| ATOM | 2765 H | GLU | S | 786 | 34.601 | 68.501 | 10.661 | 1.00 | 0.00 |
| ATOM | 2766 N | ASP | S | 787 | 31.923 | 68.029 | 10.475 | 1.00 | 0.00 |
| ATOM | 2767 CA | ASP | S | 787 | 30.963 | 66.975 | 10.132 | 1.00 | 0.00 |
| ATOM | 2768 C | ASP | S | 787 | 30.995 | 65.791 | 11.101 | 1.00 | 0.00 |
| ATOM | 2769 O | ASP | S | 787 | 30.104 | 65.591 | 11.920 | 1.00 | 0.00 |
| ATOM | 2770 CB | ASP | S | 787 | 31.127 | 66.569 | 8.647 | 1.00 | 0.00 |
| ATOM | 2771 CG | ASP | S | 787 | 32.535 | 66.087 | 8.290 | 1.00 | 0.00 |
| ATOM | 2772 OD1 | ASP | S | 787 | 33.499 | 66.487 | 8.935 | 1.00 | 0.00 |
| ATOM | 2773 OD2 | ASP | S | 787 | 32.678 | 65.286 | 7.377 | 1.00 | 0.00 |
| ATOM | 2774 H | ASP | S | 787 | 32.644 | 68.267 | 9.819 | 1.00 | 0.00 |
| ATOM | 2775 N | LEU | S | 788 | 32.123 | 65.075 | 11.051 | 1.00 | 0.00 |
| ATOM | 2776 CA | LEU | S | 788 | 32.312 | 63.839 | 11.809 | 1.00 | 0.00 |
| ATOM | 2777 C | LEU | S | 788 | 32.431 | 64.010 | 13.311 | 1.00 | 0.00 |
| ATOM | 2778 O | LEU | S | 788 | 32.365 | 63.058 | 14.090 | 1.00 | 0.00 |
| ATOM | 2779 CB | LEU | S | 788 | 33.570 | 63.123 | 11.315 | 1.00 | 0.00 |
| ATOM | 2780 CG | LEU | S | 788 | 33.765 | 63.083 | 9.797 | 1.00 | 0.00 |
| ATOM | 2781 CD1 | LEU | S | 788 | 35.108 | 62.463 | 9.432 | 1.00 | 0.00 |
| ATOM | 2782 CD2 | LEU | S | 788 | 32.603 | 62.428 | 9.052 | 1.00 | 0.00 |
| ATOM | 2783 H | LEU | S | 788 | 32.779 | 65.333 | 10.342 | 1.00 | 0.00 |
| ATOM | 2784 N | ASP | S | 789 | 32.687 | 65.268 | 13.694 | 1.00 | 0.00 |
| ATOM | 2785 CA | ASP | S | 789 | 32.897 | 65.416 | 15.121 | 1.00 | 0.00 |
| ATOM | 2786 C | ASP | S | 789 | 31.662 | 65.801 | 15.903 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2787 O | ASP | S | 789 | 31.021 | 64.963 | 16.549 | 1.00 | 0.00 |
| ATOM | 2788 CB | ASP | S | 789 | 34.100 | 66.321 | 15.438 | 1.00 | 0.00 |
| ATOM | 2789 CG | ASP | S | 789 | 34.738 | 65.956 | 16.775 | 1.00 | 0.00 |
| ATOM | 2790 OD1 | ASP | S | 789 | 34.472 | 64.834 | 17.294 | 1.00 | 0.00 |
| ATOM | 2791 OD2 | ASP | S | 789 | 35.522 | 66.726 | 17.315 | 1.00 | 0.00 |
| ATOM | 2792 H | ASP | S | 789 | 32.665 | 66.048 | 13.071 | 1.00 | 0.00 |
| ATOM | 2793 N | LYS | S | 790 | 31.392 | 67.114 | 15.894 | 1.00 | 0.00 |
| ATOM | 2794 CA | LYS | S | 790 | 30.651 | 67.706 | 17.017 | 1.00 | 0.00 |
| ATOM | 2795 C | LYS | S | 790 | 29.331 | 67.053 | 17.341 | 1.00 | 0.00 |
| ATOM | 2796 O | LYS | S | 790 | 29.016 | 66.704 | 18.482 | 1.00 | 0.00 |
| ATOM | 2797 CB | LYS | S | 790 | 30.393 | 69.191 | 16.800 | 1.00 | 0.00 |
| ATOM | 2798 CG | LYS | S | 790 | 31.625 | 69.956 | 16.346 | 1.00 | 0.00 |
| ATOM | 2799 CD | LYS | S | 790 | 32.764 | 70.041 | 17.363 | 1.00 | 0.00 |
| ATOM | 2800 CE | LYS | S | 790 | 33.927 | 70.843 | 16.777 | 1.00 | 0.00 |
| ATOM | 2801 NZ | LYS | S | 790 | 33.407 | 72.128 | 16.290 | 1.00 | 0.00 |
| ATOM | 2802 H | LYS | S | 790 | 31.859 | 67.701 | 15.232 | 1.00 | 0.00 |
| ATOM | 2803 1HZ | LYS | S | 790 | 33.058 | 72.737 | 17.054 | 1.00 | 0.00 |
| ATOM | 2804 2HZ | LYS | S | 790 | 32.631 | 71.963 | 15.612 | 1.00 | 0.00 |
| ATOM | 2805 3HZ | LYS | S | 790 | 34.104 | 72.634 | 15.713 | 1.00 | 0.00 |
| ATOM | 2806 N | THR | S | 791 | 28.592 | 66.873 | 16.238 | 1.00 | 0.00 |
| ATOM | 2807 CA | THR | S | 791 | 27.173 | 66.532 | 16.242 | 1.00 | 0.00 |
| ATOM | 2808 C | THR | S | 791 | 26.774 | 65.165 | 16.828 | 1.00 | 0.00 |
| ATOM | 2809 O | THR | S | 791 | 25.611 | 64.802 | 17.015 | 1.00 | 0.00 |
| ATOM | 2810 CB | THR | S | 791 | 26.678 | 66.834 | 14.814 | 1.00 | 0.00 |
| ATOM | 2811 OG1 | THR | S | 791 | 25.265 | 67.032 | 14.757 | 1.00 | 0.00 |
| ATOM | 2812 CG2 | THR | S | 791 | 27.163 | 65.832 | 13.769 | 1.00 | 0.00 |
| ATOM | 2813 H | THR | S | 791 | 29.033 | 67.136 | 15.379 | 1.00 | 0.00 |
| ATOM | 2814 HG1 | THR | S | 791 | 25.052 | 67.421 | 13.911 | 1.00 | 0.00 |
| ATOM | 2815 N | TRP | S | 792 | 27.810 | 64.408 | 17.236 | 1.00 | 0.00 |
| ATOM | 2816 CA | TRP | S | 792 | 27.477 | 63.320 | 18.153 | 1.00 | 0.00 |
| ATOM | 2817 C | TRP | S | 792 | 26.909 | 63.743 | 19.509 | 1.00 | 0.00 |
| ATOM | 2818 O | TRP | S | 792 | 26.105 | 63.043 | 20.129 | 1.00 | 0.00 |
| ATOM | 2819 CB | TRP | S | 792 | 28.642 | 62.345 | 18.338 | 1.00 | 0.00 |
| ATOM | 2820 CG | TRP | S | 792 | 28.101 | 61.135 | 19.064 | 1.00 | 0.00 |
| ATOM | 2821 CD1 | TRP | S | 792 | 27.313 | 60.120 | 18.506 | 1.00 | 0.00 |
| ATOM | 2822 CD2 | TRP | S | 792 | 28.204 | 60.816 | 20.470 | 1.00 | 0.00 |
| ATOM | 2823 NE1 | TRP | S | 792 | 26.928 | 59.223 | 19.448 | 1.00 | 0.00 |
| ATOM | 2824 CE2 | TRP | S | 792 | 27.452 | 59.611 | 20.681 | 1.00 | 0.00 |
| ATOM | 2825 CE3 | TRP | S | 792 | 28.853 | 61.446 | 21.554 | 1.00 | 0.00 |
| ATOM | 2826 CZ2 | TRP | S | 792 | 27.365 | 59.068 | 21.980 | 1.00 | 0.00 |
| ATOM | 2827 CZ3 | TRP | S | 792 | 28.757 | 60.888 | 22.846 | 1.00 | 0.00 |
| ATOM | 2828 CH2 | TRP | S | 792 | 28.016 | 59.706 | 23.059 | 1.00 | 0.00 |
| ATOM | 2829 H | TRP | S | 792 | 28.735 | 64.658 | 16.948 | 1.00 | 0.00 |
| ATOM | 2830 HE1 | TRP | S | 792 | 26.385 | 58.426 | 19.209 | 1.00 | 0.00 |
| ATOM | 2831 N | VAL | S | 793 | 27.346 | 64.915 | 19.983 | 1.00 | 0.00 |
| ATOM | 2832 CA | VAL | S | 793 | 26.567 | 65.557 | 21.052 | 1.00 | 0.00 |
| ATOM | 2833 C | VAL | S | 793 | 25.797 | 66.710 | 20.433 | 1.00 | 0.00 |
| ATOM | 2834 O | VAL | S | 793 | 25.621 | 66.694 | 19.218 | 1.00 | 0.00 |
| ATOM | 2835 CB | VAL | S | 793 | 27.455 | 65.972 | 22.235 | 1.00 | 0.00 |
| ATOM | 2836 CG1 | VAL | S | 793 | 27.742 | 64.762 | 23.125 | 1.00 | 0.00 |
| ATOM | 2837 CG2 | VAL | S | 793 | 28.744 | 66.661 | 21.795 | 1.00 | 0.00 |
| ATOM | 2838 H | VAL | S | 793 | 28.012 | 65.435 | 19.448 | 1.00 | 0.00 |
| ATOM | 2839 N | ARG | S | 794 | 25.328 | 67.677 | 21.235 | 1.00 | 0.00 |
| ATOM | 2840 CA | ARG | S | 794 | 24.867 | 68.902 | 20.584 | 1.00 | 0.00 |
| ATOM | 2841 C | ARG | S | 794 | 26.064 | 69.738 | 20.131 | 1.00 | 0.00 |
| ATOM | 2842 O | ARG | S | 794 | 26.420 | 69.733 | 18.957 | 1.00 | 0.00 |
| ATOM | 2843 CB | ARG | S | 794 | 23.853 | 69.647 | 21.476 | 1.00 | 0.00 |
| ATOM | 2844 CG | ARG | S | 794 | 22.677 | 68.755 | 21.925 | 1.00 | 0.00 |
| ATOM | 2845 CD | ARG | S | 794 | 21.743 | 69.405 | 22.962 | 1.00 | 0.00 |
| ATOM | 2846 NE | ARG | S | 794 | 20.944 | 68.410 | 23.691 | 1.00 | 0.00 |
| ATOM | 2847 CZ | ARG | S | 794 | 21.075 | 68.246 | 25.033 | 1.00 | 0.00 |
| ATOM | 2848 NH1 | ARG | S | 794 | 20.364 | 67.307 | 25.642 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2849 NH2 | ARG | S | 794 | 21.880 | 69.022 | 25.747 | 1.00 | 0.00 |
| ATOM | 2850 H | ARG | S | 794 | 25.342 | 67.603 | 22.232 | 1.00 | 0.00 |
| ATOM | 2851 HE | ARG | S | 794 | 20.258 | 67.859 | 23.222 | 1.00 | 0.00 |
| ATOM | 2852 1HH1 | ARG | S | 794 | 20.534 | 67.113 | 26.601 | 1.00 | 0.00 |
| ATOM | 2853 2HH1 | ARG | S | 794 | 19.670 | 66.758 | 25.171 | 1.00 | 0.00 |
| ATOM | 2854 1HH2 | ARG | S | 794 | 21.806 | 69.122 | 26.737 | 1.00 | 0.00 |
| ATOM | 2855 2HH2 | ARG | S | 794 | 22.618 | 69.509 | 25.285 | 1.00 | 0.00 |
| ATOM | 2856 N | TYR | S | 795 | 26.738 | 70.371 | 21.110 | 1.00 | 0.00 |
| ATOM | 2857 CA | TYR | S | 795 | 28.061 | 70.869 | 20.744 | 1.00 | 0.00 |
| ATOM | 2858 C | TYR | S | 795 | 29.170 | 70.261 | 21.587 | 1.00 | 0.00 |
| ATOM | 2859 O | TYR | S | 795 | 29.980 | 69.482 | 21.098 | 1.00 | 0.00 |
| ATOM | 2860 CB | TYR | S | 795 | 28.109 | 72.405 | 20.711 | 1.00 | 0.00 |
| ATOM | 2861 CG | TYR | S | 795 | 29.405 | 72.853 | 20.070 | 1.00 | 0.00 |
| ATOM | 2862 CD1 | TYR | S | 795 | 30.473 | 73.232 | 20.907 | 1.00 | 0.00 |
| ATOM | 2863 CD2 | TYR | S | 795 | 29.526 | 72.856 | 18.664 | 1.00 | 0.00 |
| ATOM | 2864 CE1 | TYR | S | 795 | 31.708 | 73.563 | 20.333 | 1.00 | 0.00 |
| ATOM | 2865 CE2 | TYR | S | 795 | 30.760 | 73.201 | 18.087 | 1.00 | 0.00 |
| ATOM | 2866 CZ | TYR | S | 795 | 31.841 | 73.530 | 18.931 | 1.00 | 0.00 |
| ATOM | 2867 OH | TYR | S | 795 | 33.075 | 73.831 | 18.384 | 1.00 | 0.00 |
| ATOM | 2868 H | TYR | S | 795 | 26.390 | 70.380 | 22.044 | 1.00 | 0.00 |
| ATOM | 2869 HH | TYR | S | 795 | 33.698 | 73.706 | 19.100 | 1.00 | 0.00 |
| ATOM | 2870 N | GLN | S | 796 | 29.160 | 70.624 | 22.878 | 1.00 | 0.00 |
| ATOM | 2871 CA | GLN | S | 796 | 30.089 | 69.997 | 23.825 | 1.00 | 0.00 |
| ATOM | 2872 C | GLN | S | 796 | 29.392 | 69.725 | 25.149 | 1.00 | 0.00 |
| ATOM | 2873 O | GLN | S | 796 | 29.767 | 70.163 | 26.238 | 1.00 | 0.00 |
| ATOM | 2874 CB | GLN | S | 796 | 31.397 | 70.804 | 23.938 | 1.00 | 0.00 |
| ATOM | 2875 CG | GLN | S | 796 | 31.221 | 72.301 | 24.201 | 1.00 | 0.00 |
| ATOM | 2876 CD | GLN | S | 796 | 32.503 | 73.076 | 23.922 | 1.00 | 0.00 |
| ATOM | 2877 OE1 | GLN | S | 796 | 33.364 | 72.711 | 23.129 | 1.00 | 0.00 |
| ATOM | 2878 NE2 | GLN | S | 796 | 32.548 | 74.267 | 24.499 | 1.00 | 0.00 |
| ATOM | 2879 H | GLN | S | 796 | 28.493 | 71.289 | 23.218 | 1.00 | 0.00 |
| ATOM | 2880 1HE2 | GLN | S | 796 | 33.127 | 75.023 | 24.202 | 1.00 | 0.00 |
| ATOM | 2881 2HE2 | GLN | S | 796 | 31.952 | 74.368 | 25.305 | 1.00 | 0.00 |
| ATOM | 2882 N | GLU | S | 797 | 28.279 | 68.987 | 24.961 | 1.00 | 0.00 |
| ATOM | 2883 CA | GLU | S | 797 | 27.163 | 68.939 | 25.902 | 1.00 | 0.00 |
| ATOM | 2884 C | GLU | S | 797 | 27.038 | 69.942 | 27.033 | 1.00 | 0.00 |
| ATOM | 2885 O | GLU | S | 797 | 26.907 | 71.131 | 26.755 | 1.00 | 0.00 |
| ATOM | 2886 CB | GLU | S | 797 | 26.752 | 67.505 | 26.247 | 1.00 | 0.00 |
| ATOM | 2887 CG | GLU | S | 797 | 25.220 | 67.443 | 26.277 | 1.00 | 0.00 |
| ATOM | 2888 CD | GLU | S | 797 | 24.699 | 67.911 | 24.932 | 1.00 | 0.00 |
| ATOM | 2889 OE1 | GLU | S | 797 | 24.596 | 67.085 | 24.041 | 1.00 | 0.00 |
| ATOM | 2890 OE2 | GLU | S | 797 | 24.422 | 69.099 | 24.751 | 1.00 | 0.00 |
| ATOM | 2891 H | GLU | S | 797 | 28.177 | 68.606 | 24.043 | 1.00 | 0.00 |
| ATOM | 2892 N | CYS | S | 798 | 27.060 | 69.446 | 28.273 | 1.00 | 0.00 |
| ATOM | 2893 CA | CYS | S | 798 | 26.843 | 70.326 | 29.415 | 1.00 | 0.00 |
| ATOM | 2894 C | CYS | S | 798 | 28.111 | 71.069 | 29.843 | 1.00 | 0.00 |
| ATOM | 2895 O | CYS | S | 798 | 28.191 | 71.556 | 30.966 | 1.00 | 0.00 |
| ATOM | 2896 CB | CYS | S | 798 | 26.251 | 69.427 | 30.510 | 1.00 | 0.00 |
| ATOM | 2897 SG | CYS | S | 798 | 25.036 | 69.994 | 31.753 | 1.00 | 0.00 |
| ATOM | 2898 H | CYS | S | 798 | 27.164 | 68.446 | 28.416 | 1.00 | 0.00 |
| ATOM | 2899 N | ASP | S | 799 | 29.083 | 71.105 | 28.904 | 1.00 | 0.00 |
| ATOM | 2900 CA | ASP | S | 799 | 30.385 | 71.757 | 29.015 | 1.00 | 0.00 |
| ATOM | 2901 C | ASP | S | 799 | 31.300 | 71.400 | 30.152 | 1.00 | 0.00 |
| ATOM | 2902 O | ASP | S | 799 | 30.907 | 71.046 | 31.254 | 1.00 | 0.00 |
| ATOM | 2903 CB | ASP | S | 799 | 30.331 | 73.263 | 28.787 | 1.00 | 0.00 |
| ATOM | 2904 CG | ASP | S | 799 | 31.123 | 73.573 | 27.531 | 1.00 | 0.00 |
| ATOM | 2905 OD1 | ASP | S | 799 | 30.658 | 74.403 | 26.753 | 1.00 | 0.00 |
| ATOM | 2906 OD2 | ASP | S | 799 | 32.186 | 72.978 | 27.306 | 1.00 | 0.00 |
| ATOM | 2907 H | ASP | S | 799 | 28.899 | 70.638 | 28.050 | 1.00 | 0.00 |
| ATOM | 2908 N | SER | S | 800 | 32.581 | 71.425 | 29.814 | 1.00 | 0.00 |
| ATOM | 2909 CA | SER | S | 800 | 33.531 | 70.826 | 30.736 | 1.00 | 0.00 |
| ATOM | 2910 C | SER | S | 800 | 34.469 | 71.819 | 31.362 | 1.00 | 0.00 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2911 O | SER | S | 800 | 35.683 | 71.822 | 31.144 | 1.00 | 0.00 |
| ATOM | 2912 CB | SER | S | 800 | 34.293 | 69.706 | 30.057 | 1.00 | 0.00 |
| ATOM | 2913 OG | SER | S | 800 | 33.374 | 68.760 | 29.495 | 1.00 | 0.00 |
| ATOM | 2914 H | SER | S | 800 | 32.816 | 71.967 | 29.008 | 1.00 | 0.00 |
| ATOM | 2915 HG | SER | S | 800 | 33.406 | 68.383 | 28.546 | 1.00 | 0.00 |
| ATOM | 2916 N | ARG | S | 801 | 33.858 | 72.682 | 32.173 | 1.00 | 0.00 |
| ATOM | 2917 CA | ARG | S | 801 | 34.693 | 73.709 | 32.776 | 1.00 | 0.00 |
| ATOM | 2918 C | ARG | S | 801 | 34.278 | 74.080 | 34.185 | 1.00 | 0.00 |
| ATOM | 2919 O | ARG | S | 801 | 33.912 | 75.216 | 34.491 | 1.00 | 0.00 |
| ATOM | 2920 CB | ARG | S | 801 | 34.798 | 74.942 | 31.862 | 1.00 | 0.00 |
| ATOM | 2921 CG | ARG | S | 801 | 36.130 | 75.707 | 31.952 | 1.00 | 0.00 |
| ATOM | 2922 CD | ARG | S | 801 | 37.288 | 75.182 | 31.075 | 1.00 | 0.00 |
| ATOM | 2923 NE | ARG | S | 801 | 37.651 | 73.793 | 31.363 | 1.00 | 0.00 |
| ATOM | 2924 CZ | ARG | S | 801 | 38.461 | 73.469 | 32.394 | 1.00 | 0.00 |
| ATOM | 2925 NH1 | ARG | S | 801 | 38.546 | 72.215 | 32.807 | 1.00 | 0.00 |
| ATOM | 2926 NH2 | ARG | S | 801 | 39.156 | 74.399 | 33.026 | 1.00 | 0.00 |
| ATOM | 2927 H | ARG | S | 801 | 32.858 | 72.662 | 32.275 | 1.00 | 0.00 |
| ATOM | 2928 HE | ARG | S | 801 | 37.190 | 73.050 | 30.867 | 1.00 | 0.00 |
| ATOM | 2929 1HH1 | ARG | S | 801 | 39.159 | 72.001 | 33.585 | 1.00 | 0.00 |
| ATOM | 2930 2HH1 | ARG | S | 801 | 38.017 | 71.466 | 32.402 | 1.00 | 0.00 |
| ATOM | 2931 1HH2 | ARG | S | 801 | 39.638 | 74.139 | 33.871 | 1.00 | 0.00 |
| ATOM | 2932 2HH2 | ARG | S | 801 | 39.224 | 75.336 | 32.697 | 1.00 | 0.00 |
| ATOM | 2933 N | SER | S | 802 | 34.427 | 73.084 | 35.072 | 1.00 | 0.00 |
| ATOM | 2934 CA | SER | S | 802 | 34.174 | 73.382 | 36.483 | 1.00 | 0.00 |
| ATOM | 2935 C | SER | S | 802 | 35.119 | 74.346 | 37.166 | 1.00 | 0.00 |
| ATOM | 2936 O | SER | S | 802 | 34.974 | 74.647 | 38.347 | 1.00 | 0.00 |
| ATOM | 2937 CB | SER | S | 802 | 34.094 | 72.100 | 37.279 | 1.00 | 0.00 |
| ATOM | 2938 OG | SER | S | 802 | 33.450 | 71.146 | 36.438 | 1.00 | 0.00 |
| ATOM | 2939 H | SER | S | 802 | 34.664 | 72.146 | 34.807 | 1.00 | 0.00 |
| ATOM | 2940 HG | SER | S | 802 | 32.501 | 71.240 | 36.590 | 1.00 | 0.00 |
| ATOM | 2941 N | ASN | S | 803 | 36.053 | 74.872 | 36.354 | 1.00 | 0.00 |
| ATOM | 2942 CA | ASN | S | 803 | 36.802 | 76.102 | 36.625 | 1.00 | 0.00 |
| ATOM | 2943 C | ASN | S | 803 | 38.031 | 75.957 | 37.488 | 1.00 | 0.00 |
| ATOM | 2944 O | ASN | S | 803 | 39.095 | 76.508 | 37.221 | 1.00 | 0.00 |
| ATOM | 2945 CB | ASN | S | 803 | 35.911 | 77.251 | 37.104 | 1.00 | 0.00 |
| ATOM | 2946 CG | ASN | S | 803 | 36.069 | 78.395 | 36.138 | 1.00 | 0.00 |
| ATOM | 2947 OD1 | ASN | S | 803 | 36.832 | 79.332 | 36.342 | 1.00 | 0.00 |
| ATOM | 2948 ND2 | ASN | S | 803 | 35.315 | 78.283 | 35.038 | 1.00 | 0.00 |
| ATOM | 2949 H | ASN | S | 803 | 36.303 | 74.295 | 35.579 | 1.00 | 0.00 |
| ATOM | 2950 1HD2 | ASN | S | 803 | 34.680 | 77.519 | 34.912 | 1.00 | 0.00 |
| ATOM | 2951 2HD2 | ASN | S | 803 | 35.408 | 78.968 | 34.320 | 1.00 | 0.00 |
| ATOM | 2952 N | ALA | S | 804 | 37.877 | 75.156 | 38.544 | 1.00 | 0.00 |
| ATOM | 2953 CA | ALA | S | 804 | 39.112 | 74.680 | 39.156 | 1.00 | 0.00 |
| ATOM | 2954 C | ALA | S | 804 | 39.890 | 73.646 | 38.331 | 1.00 | 0.00 |
| ATOM | 2955 O | ALA | S | 804 | 41.058 | 73.888 | 38.052 | 1.00 | 0.00 |
| ATOM | 2956 CB | ALA | S | 804 | 38.897 | 74.236 | 40.613 | 1.00 | 0.00 |
| ATOM | 2957 H | ALA | S | 804 | 36.982 | 74.726 | 38.623 | 1.00 | 0.00 |
| ATOM | 2958 N | PRO | S | 805 | 39.247 | 72.508 | 37.945 | 1.00 | 0.00 |
| ATOM | 2959 CA | PRO | S | 805 | 40.013 | 71.526 | 37.176 | 1.00 | 0.00 |
| ATOM | 2960 C | PRO | S | 805 | 39.936 | 71.786 | 35.669 | 1.00 | 0.00 |
| ATOM | 2961 O | PRO | S | 805 | 39.664 | 72.906 | 35.258 | 1.00 | 0.00 |
| ATOM | 2962 CB | PRO | S | 805 | 39.317 | 70.232 | 37.604 | 1.00 | 0.00 |
| ATOM | 2963 CG | PRO | S | 805 | 37.838 | 70.613 | 37.667 | 1.00 | 0.00 |
| ATOM | 2964 CD | PRO | S | 805 | 37.881 | 72.039 | 38.197 | 1.00 | 0.00 |
| ATOM | 2965 OXT | PRO | S | 805 | 40.122 | 70.862 | 34.884 | 1.00 | 0.00 |
| ATOM | 2966 C1 | GLYC | G | 1 | 29.245 | 53.000 | 28.747 | 1.00 | 0.00 |
| ATOM | 2967 C2 | GLYC | G | 1 | 30.276 | 51.881 | 28.832 | 1.00 | 0.00 |
| ATOM | 2968 O1 | GLYC | G | 1 | 30.006 | 50.867 | 29.448 | 1.00 | 0.00 |
| ATOM | 2969 O2 | GLYC | G | 1 | 31.330 | 51.994 | 28.220 | 1.00 | 0.00 |
| ATOM | 2970 N1 | GLYC | G | 1 | 29.000 | 53.157 | 27.339 | 1.00 | 0.00 |
| ATOM | 2971 3H | GLYC | G | 1 | 29.637 | 53.933 | 29.148 | 1.00 | 0.00 |
| ATOM | 2972 4H | GLYC | G | 1 | 28.716 | 54.113 | 27.090 | 1.00 | 0.00 |

```
ATOM   2973 5H   GLYC  G    1      28.318   52.450   26.998   1.00   0.00
ATOM   2974 1H   GLYC  G    1      29.926   52.936   26.928   1.00   0.00
ATOM   2975 2H   GLYC  G    1      28.317   52.742   29.258   1.00   0.00
END
```

Publications cited herein and the material for which they are cited are specifically incorporated by reference.

Those skilled in the art will recognize, or be able to ascertain using no more than routine experimentation, many equivalents to the specific embodiments of the invention described herein. Such equivalents are intended to be encompassed by the following claims.

SEQUENCE LISTING

(1) GENERAL INFORMATION:
(i) APPLICANT: Bearsden Bio, Inc.
(ii) TITLE OF INVENTION: METHOD OF DETERMINING PROTEIN-LIGAND INTERACTIONS VIA COMPUTER MODELING

(iii) NUMBER OF SEQUENCES: 25

(iv) CORRESPONDENCE ADDRESS:
(A) ADDRESSEE: Patrea L. Pabst
(B) STREET: 2800 One Atlantic Center
1201 West Peachtree Street
(C) CITY: Atlanta
(D) STATE: Georgia
(E) COUNTRY: USA
(F) ZIP: 30306-3450

(v) COMPUTER READABLE FORM:
(A) MEDIUM TYPE: Floppy disk
(B) COMPUTER: IBM PC compatible
(C) OPERATING SYSTEM: PC-DOS/MS-DOS
(D) SOFTWARE: PatentIn Release #1.0, Version #1.25

(vi) CURRENT APPLICATION DATA:
(A) APPLICATION NUMBER: PCT/US98/03951
(B) FILING DATE: February 27, 1998
(C) CLASSIFICATION:

(viii) ATTORNEY/AGENT INFORMATION:
(A) NAME: Pabst, Patrea L.
(B) REGISTRATION NUMBER: 31,284
(C) REFERENCE/DOCKET NUMBER: SYM111

(ix) TELECOMMUNICATION INFORMATION:
(A) TELEPHONE: (404)873-8794
(B) TELEFAX: (404)873-8795

(2) INFORMATION FOR SEQ ID NO:1:
(i) SEQUENCE CHARACTERISTICS:
(A) LENGTH: 238 amino acids
(B) TYPE: amino acid
(C) STRANDEDNESS: single
(D) TOPOLOGY: linear
(ii) MOLECULE TYPE: protein
(iii) HYPOTHETICAL: NO
(iv) ANTI-SENSE: NO
(xi) SEQUENCE DESCRIPTION: SEQ ID NO:1:

```
Ala Leu Pro Asp Thr Val Arg Ile Gly Thr Asp Thr Thr Tyr Ala Pro
1               5                  10                  15

Phe Ser Ser Lys Asp Ala Lys Gly Glu Phe Ile Gly Phe Asp Ile Asp
            20                  25                  30

Leu Gly Asn Glu Met Cys Lys Arg Met Gln Val Lys Cys Thr Trp Val
        35                  40                  45

Ala Ser Asp Phe Asp Ala Leu Ile Pro Ser Leu Lys Ala Lys Lys Ile
    50                  55                  60

Asp Ala Ile Ile Ser Ser Leu Ser Ile Thr Asp Lys Arg Gln Gln Glu
65                  70                  75                  80

Ile Ala Phe Ser Asp Lys Leu Tyr Ala Ala Asp Ser Arg Leu Ile Ala
                85                  90                  95
```

```
Ala Lys Gly Ser Pro Val Gln Pro Thr Leu Glu Ser Leu Lys Gly Lys
            100                 105                 110

His Val Gly Val Leu Gln Gly Ser Thr Gln Glu Ala Tyr Ala Asn Asp
        115                 120                 125

Asn Trp Arg Thr Lys Gly Val Asp Val Val Ala Tyr Ala Asn Gln Asp
    130                 135                 140

Leu Ile Tyr Ser Asp Leu Thr Ala Gly Arg Leu Asp Ala Ala Leu Gln
145                 150                 155                 160

Asp Glu Val Ala Ala Ser Glu Gly Phe Leu Lys Gln Pro Ala Gly Lys
                165                 170                 175

Glu Tyr Ala Phe Ala Gly Pro Ser Val Lys Asp Lys Lys Tyr Phe Gly
            180                 185                 190

Asp Gly Thr Gly Val Gly Leu Arg Lys Asp Asp Thr Glu Leu Lys Ala
        195                 200                 205

Ala Phe Asp Lys Ala Leu Thr Glu Leu Arg Gln Asp Gly Thr Tyr Asp
    210                 215                 220

Lys Met Ala Lys Lys Tyr Phe Asp Phe Asn Val Tyr Gly Asp
225                 230                 235
```

(2) INFORMATION FOR SEQ ID NO:2:

(i) SEQUENCE CHARACTERISTICS:

(A) LENGTH: 154 amino acids

(B) TYPE: amino acid

(C) STRANDEDNESS: single

(D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(iii) HYPOTHETICAL: NO

(iv) ANTI-SENSE: NO

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:2

```
Ser Thr Arg Leu Lys Ile Val Thr Ile His Gln Glu Pro Phe Val Tyr
1               5                   10                  15

Val Lys Pro Thr Leu Ser Asp Gly Thr Cys Lys Glu Glu Phe Thr Val
            20                  25                  30

Asn Gly Asp Pro Val Lys Lys Val Ile Cys Thr Gly Pro Asn Asp Thr
        35                  40                  45

Ser Pro Gly Ser Pro Arg His Thr Val Pro Gln Cys Cys Tyr Gly Phe
    50                  55                  60

Cys Ile Asp Leu Leu Ile Lys Leu Ala Arg Thr Met Asn Phe Thr Tyr
65                  70                  75                  80

Glu Val His Leu Val Ala Asp Gly Lys Phe Gly Thr Gln Glu Arg Val
                85                  90                  95

Asn Asn Ser Asn Lys Lys Glu Trp Asn Gly Met Met Gly Glu Leu Leu
            100                 105                 110

Ser Gly Gln Ala Asp Met Ile Val Ala Pro Leu Thr Ile Asn Asn Glu
        115                 120                 125

Arg Ala Gln Tyr Ile Glu Phe Ser Lys Pro Phe Lys Tyr Gln Gly Leu
    130                 135                 140

Thr Ile Leu Val Lys Lys Glu Ile Pro Arg
145                 150
```

(2) INFORMATION FOR SEQ ID NO:3:
(i) SEQUENCE CHARACTERISTICS:
(A) LENGTH: 136 amino acids
(B) TYPE: amino acid
(C) STRANDEDNESS: single
(D) TOPOLOGY: linear
(ii) MOLECULE TYPE: protein
(iii) HYPOTHETICAL: NO
(iv) ANTI-SENSE: NO
(xi) SEQUENCE DESCRIPTION: SEQ ID NO:3

```
Thr Gly Ile Asn Asp Pro Arg Leu Arg Asn Pro Ser Asp Lys Phe Ile
1               5                  10                  15

Tyr Ala Thr Val Lys Gln Ser Ser Val Asp Ile Tyr Phe Arg Arg Gln
            20                  25                  30

Val Glu Leu Ser Thr Met Tyr Arg His Met Glu Lys His Asn Tyr Glu
        35                  40                  45

Ser Ala Ala Glu Ala Ile Gln Ala Val Arg Asp Asn Lys Leu His Ala
    50                  55                  60

Phe Ile Trp Asp Ser Ala Val Leu Glu Phe Glu Ala Ser Gln Lys Cys
65                  70                  75                  80

Asp Leu Val Thr Thr Gly Glu Leu Phe Phe Arg Ser Gly Phe Gly Ile
                85                  90                  95

Gly Met Arg Lys Asp Ser Pro Trp Lys Gln Asn Val Ser Leu Ser Ile
            100                 105                 110

Leu Lys Ser His Glu Asn Gly Phe Met Glu Asp Leu Asp Lys Thr Trp
        115                 120                 125

Val Arg Tyr Gln Glu Cys Asp Ser
    130                 135
```

(2) INFORMATION FOR SEQ ID NO:4:
(i) SEQUENCE CHARACTERISTICS:
(A) LENGTH: 140 amino acids
(B) TYPE: amino acid
(C) STRANDEDNESS: single
(D) TOPOLOGY: linear
(ii) MOLECULE TYPE: protein
(iii) HYPOTHETICAL: NO
(iv) ANTI-SENSE: NO
(xi) SEQUENCE DESCRIPTION: SEQ ID NO:4

```
Ser Arg His Leu Thr Val Ala Thr Leu Glu Glu Arg Pro Phe Val Ile
1               5                  10                  15

Val Glu Ser Pro Asp Pro Gly Thr Gly Gly Cys Val Pro Asn Thr Val
            20                  25                  30

Pro Cys Arg Arg Gln Ser Asn His Thr Phe Ser Ser Gly Asp Val Ala
        35                  40                  45

Pro Tyr Thr Lys Leu Cys Cys Lys Gly Phe Cys Ile Asp Ile Leu Lys
    50                  55                  60

Lys Leu Ala Arg Val Val Lys Phe Ser Tyr Asp Leu Tyr Leu Val Thr
65                  70                  75                  80

Asn Gly Lys His Gly Lys Arg Val Arg Gly Val Trp Asn Gly Met Ile
                85                  90                  95
```

```
Gly Glu Val Tyr Tyr Lys Arg Ala Asp Met Ala Ile Gly Ser Leu Thr
            100                 105                 110

Ile Asn Glu Glu Arg Ser Glu Ile Val Asp Phe Ser Val Pro Phe Val
        115                 120                 125

Glu Thr Gly Ile Ser Val Met Val Ala Arg Ser Asn
    130                 135                 140
```

(2) INFORMATION FOR SEQ ID NO:5:

(i) SEQUENCE CHARACTERISTICS:
- (A) LENGTH: 135 amino acids
- (B) TYPE: amino acid
- (C) STRANDEDNESS: single
- (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(iii) HYPOTHETICAL: NO

(iv) ANTI-SENSE: NO

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:5

```
Lys Lys Phe Gln Arg Pro Gln Asp Gln Tyr Pro Pro Phe Arg Phe Gly
1               5                   10                  15

Thr Val Pro Asn Gly Ser Thr Glu Arg Asn Ile Arg Ser Asn Tyr Arg
            20                  25                  30

Asp Met His Thr His Met Val Lys Phe Asn Gln Arg Ser Val Glu Asp
        35                  40                  45

Ala Leu Thr Ser Leu Lys Met Gly Lys Leu Asp Ala Phe Ile Tyr Asp
    50                  55                  60

Ala Ala Val Leu Asn Tyr Met Ala Gly Lys Asp Glu Gly Cys Lys Leu
65                  70                  75                  80

Val Thr Ile Gly Ser Gly Lys Val Phe Ala Thr Thr Gly Tyr Gly Ile
                85                  90                  95

Ala Met Gln Lys Asp Ser His Trp Lys Arg Ala Ile Asp Leu Ala Leu
            100                 105                 110

Leu Gln Phe Leu Gly Asp Gly Glu Thr Gln Lys Leu Glu Thr Val Trp
        115                 120                 125

Leu Ser Gly Ile Cys Gln Asn
    130                 135
```

(2) INFORMATION FOR SEQ ID NO:6:

(i) SEQUENCE CHARACTERISTICS:
- (A) LENGTH: 140 amino acids
- (B) TYPE: amino acid
- (C) STRANDEDNESS: single
- (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(iii) HYPOTHETICAL: NO

(iv) ANTI-SENSE: NO

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:6

```
Asp Asp His Leu Ser Ile Val Thr Leu Glu Glu Ala Pro Phe Val Ile
1               5                   10                  15

Val Glu Ser Val Asp Pro Leu Ser Gly Thr Cys Met Arg Asn Thr Val
            20                  25                  30

Pro Cys Gln Lys Arg Ile Ile Ser Glu Asn Lys Thr Asp Glu Glu Pro
        35                  40                  45
```

```
Gly Tyr Ile Lys Lys Cys Cys Lys Gly Phe Cys Ile Asp Ile Leu Lys
    50                  55                  60

Lys Ile Ser Lys Ser Val Lys Phe Thr Tyr Asp Leu Tyr Leu Val Thr
65                  70                  75                  80

Asn Gly Lys His Gly Lys Lys Ile Asn Gly Thr Trp Asn Gly Met Ile
                85                  90                  95

Gly Glu Val Val Met Lys Arg Ala Tyr Met Ala Val Gly Ser Leu Thr
            100                 105                 110

Ile Asn Glu Glu Arg Ser Glu Val Val Asp Phe Ser Val Pro Phe Ile
        115                 120                 125

Glu Thr Gly Ile Ser Val Met Val Ser Arg Ser Asn
    130                 135                 140
```

(2) INFORMATION FOR SEQ ID NO:7:

(i) SEQUENCE CHARACTERISTICS:
- (A) LENGTH: 133 amino acids
- (B) TYPE: amino acid
- (C) STRANDEDNESS: single
- (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(iii) HYPOTHETICAL: NO

(iv) ANTI-SENSE: NO

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:7

```
Lys Lys Phe Gln Arg Pro Asn Asp Phe Ser Pro Pro Phe Arg Phe Gly
1               5                   10                  15

Thr Val Pro Asn Gly Ser Thr Glu Arg Asn Ile Arg Asn Asn Tyr Ala
            20                  25                  30

Glu Met His Ala Tyr Met Gly Lys Phe Asn Gln Arg Gly Val Asp Asp
        35                  40                  45

Ala Leu Leu Ser Leu Lys Thr Gly Lys Leu Asp Ala Phe Ile Tyr Asp
    50                  55                  60

Ala Ala Val Leu Asn Tyr Met Ala Gly Arg Asp Glu Gly Cys Lys Leu
65                  70                  75                  80

Val Thr Ser Gly Lys Val Phe Ala Ser Thr Gly Tyr Gly Ile Ala Ile
                85                  90                  95

Gln Lys Asp Ser Gly Trp Lys Arg Gln Val Asp Leu Ala Ile Leu Gln
            100                 105                 110

Leu Phe Gly Asp Gly Glu Met Glu Glu Leu Glu Ala Leu Trp Leu Thr
        115                 120                 125

Gly Ile Cys His Asn
    130
```

(2) INFORMATION FOR SEQ ID NO:8:

(i) SEQUENCE CHARACTERISTICS:
- (A) LENGTH: 142 amino acids
- (B) TYPE: amino acid
- (C) STRANDEDNESS: single
- (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(iii) HYPOTHETICAL: NO

(iv) ANTI-SENSE: NO

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:8

```
Asp Asn His Leu Ser Ile Val Thr Leu Glu Glu Ala Pro Phe Val Ile
1               5                  10                  15

Val Glu Asp Ile Asp Pro Leu Thr Glu Thr Cys Val Arg Asn Thr Val
            20                  25                  30

Pro Cys Arg Lys Phe Val Lys Ile Asn Asn Ser Thr Asn Glu Gly Met
        35                  40                  45

Asn Val Lys Lys Cys Cys Lys Gly Phe Cys Ile Asp Ile Leu Lys Lys
    50                  55                  60

Leu Ser Arg Thr Val Lys Phe Thr Tyr Asp Leu Tyr Leu Val Thr Asn
65                  70                  75                  80

Gly Lys His Gly Lys Lys Val Asn Asn Val Trp Asn Gly Met Ile Gly
                85                  90                  95

Glu Val Val Tyr Gln Arg Ala Val Met Ala Val Gly Ser Leu Thr Ile
            100                 105                 110

Asn Glu Glu Arg Ser Glu Val Val Asp Phe Ser Val Pro Phe Val Glu
        115                 120                 125

Thr Gly Ile Ser Val Met Val Ser Arg Ser Asn Gly Thr Val
    130                 135                 140
```

(2) INFORMATION FOR SEQ ID NO:9:
  (i) SEQUENCE CHARACTERISTICS:
    (A) LENGTH: 135 amino acids
    (B) TYPE: amino acid
    (C) STRANDEDNESS: single
    (D) TOPOLOGY: linear
  (ii) MOLECULE TYPE: protein
  (iii) HYPOTHETICAL: NO
  (iv) ANTI-SENSE: NO
  (xi) SEQUENCE DESCRIPTION: SEQ ID NO:9

```
Lys Lys Phe Gln Arg Pro His Asp Tyr Ser Pro Pro Phe Arg Phe Gly
1               5                  10                  15

Thr Val Pro Asn Gly Ser Thr Glu Arg Asn Ile Arg Asn Asn Tyr Pro
            20                  25                  30

Tyr Met His Gln Tyr Met Thr Arg Phe Asn Gln Arg Gly Val Glu Asp
        35                  40                  45

Ala Leu Val Ser Leu Lys Thr Gly Lys Leu Asp Ala Phe Ile Tyr Asp
    50                  55                  60

Ala Ala Val Leu Asn Tyr Lys Ala Gly Arg Asp Glu Gly Cys Lys Leu
65                  70                  75                  80

Val Thr Ile Gly Ser Gly Tyr Ile Phe Ala Ser Thr Gly Tyr Gly Ile
                85                  90                  95

Ala Leu Gln Lys Gly Ser Pro Trp Lys Arg Gln Ile Asp Leu Ala Leu
            100                 105                 110

Leu Gln Phe Val Gly Asp Gly Glu Met Glu Glu Leu Glu Thr Leu Trp
        115                 120                 125

Leu Thr Gly Ile Cys His Asn
    130                 135
```

(2) INFORMATION FOR SEQ ID NO:10:
(i) SEQUENCE CHARACTERISTICS:
(A) LENGTH: 123 amino acids
(B) TYPE: amino acid
(C) STRANDEDNESS: single
(D) TOPOLOGY: linear
(ii) MOLECULE TYPE: protein
(iii) HYPOTHETICAL: NO
(iv) ANTI-SENSE: NO
(xi) SEQUENCE DESCRIPTION: SEQ ID NO:10

```
Ser Ser Glu Asn Arg Thr Ile Val Val Thr Thr Ile Leu Glu Ser Pro
1               5                  10                  15

Tyr Val Met Tyr Lys Lys Asn His Glu Met Leu Glu Gly Asn Glu Arg
            20                  25                  30

Tyr Glu Gly Tyr Cys Val Asp Leu Ala Tyr Glu Ile Ala Lys His Val
        35                  40                  45

Arg Ile Lys Tyr Lys Leu Ser Ile Val Gly Asp Gly Lys Tyr Gly Ala
    50                  55                  60

Arg Asp Pro Glu Thr Lys Ile Trp Asn Gly Met Val Gly Glu Leu Val
65                  70                  75                  80

Tyr Gly Lys Ala Asp Ile Ala Val Ala Pro Leu Thr Ile Thr Leu Val
                85                  90                  95

Arg Glu Glu Val Ile Asp Phe Ser Lys Pro Phe Met Ser Leu Gly Ile
            100                 105                 110

Ser Ile Met Ile Lys Lys Pro Gln Lys Ser Lys
        115                 120
```

(2) INFORMATION FOR SEQ ID NO:11:
(i) SEQUENCE CHARACTERISTICS:
(A) LENGTH: 150 amino acids
(B) TYPE: amino acid
(C) STRANDEDNESS: single
(D) TOPOLOGY: linear
(ii) MOLECULE TYPE: protein
(iii) HYPOTHETICAL: NO
(iv) ANTI-SENSE: NO
(xi) SEQUENCE DESCRIPTION: SEQ ID NO:11

```
*Val Glu Arg Met Val Ser Pro Ile Glu Ser Ala Glu Asp Leu Ala Lys
1               5                  10                  15

Gln Glu Thr Ile Ala Tyr Gly Thr Leu Asp Ser Gly Ser Thr Lys Glu
            20                  25                  30

Phe Phe Arg Arg Ser Lys Ile Ala Val Tyr Glu Lys Met Trp Ser Tyr
        35                  40                  45

Met Lys Ser Ala Glu Pro Ser Val Phe Thr Lys Thr Thr Ala Asp Gly
    50                  55                  60

Val Ala Arg Val Arg Lys Ser Lys Gly Lys Phe Ala Phe Leu Leu Glu
65                  70                  75                  80

Ser Thr Met Asn Glu Tyr Ile Glu Gln Arg Lys Pro Cys Asp Thr Met
                85                  90                  95

Lys Val Gly Gly Asn Leu Asp Ser Lys Gly Tyr Gly Val Ala Thr Pro
            100                 105                 110
```

```
Lys Gly Ser Ala Leu Gly Asn Ala Val Asn Leu Ala Val Leu Lys Leu
        115                 120                 125

Asn Glu Gln Gly Leu Leu Asp Lys Leu Lys Asn Lys Trp Trp Tyr Asp
    130                 135                 140

Lys Gly Glu Cys Gly Ser
145                 150
```

(2) INFORMATION FOR SEQ ID NO:12:

(i) SEQUENCE CHARACTERISTICS:
- (A) LENGTH: 123 amino acids
- (B) TYPE: amino acid
- (C) STRANDEDNESS: single
- (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(iii) HYPOTHETICAL: NO

(iv) ANTI-SENSE: NO

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:12

```
Ser Leu Ser Asn Arg Ser Leu Ile Val Thr Thr Ile Leu Glu Glu Pro
1               5                   10                  15

Tyr Val Leu Phe Lys Lys Ser Asp Lys Pro Leu Tyr Gly Asn Asp Arg
            20                  25                  30

Phe Glu Gly Tyr Cys Ile Asp Leu Leu Arg Glu Leu Ser Thr Ile Leu
        35                  40                  45

Gly Phe Thr Tyr Glu Ile Arg Leu Val Glu Asp Gly Lys Tyr Gly Ala
    50                  55                  60

Gln Asp Asp Val Asn Gly Gln Trp Asn Gly Met Val Arg Glu Leu Ile
65                  70                  75                  80

Asp His Lys Ala Asp Leu Ala Val Ala Pro Leu Ala Ile Thr Tyr Val
                85                  90                  95

Arg Glu Lys Val Ile Asp Phe Ser Lys Pro Phe Met Thr Leu Gly Ile
            100                 105                 110

Ser Ile Leu Tyr Arg Lys Pro Asn Gly Thr Asn
        115                 120
```

(2) INFORMATION FOR SEQ ID NO:13:

(i) SEQUENCE CHARACTERISTICS:
- (A) LENGTH: 146 amino acids
- (B) TYPE: amino acid
- (C) STRANDEDNESS: single
- (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(iii) HYPOTHETICAL: NO

(iv) ANTI-SENSE: NO

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:13

```
Val Glu Arg Met Glu Ser Pro Ile Asp Ser Ala Asp Asp Leu Ala Lys
1               5                   10                  15

Gln Thr Lys Ile Glu Tyr Gly Ala Val Glu Asp Gly Ala Thr Met Thr
            20                  25                  30

Phe Phe Lys Lys Ser Lys Ile Ser Thr Tyr Asp Lys Met Trp Ala Phe
        35                  40                  45

Met Ser Ser Arg Arg Gln Ser Val Leu Val Lys Ser Asn Glu Glu Gly
    50                  55                  60
```

```
Ile Gln Arg Val Leu Thr Ser Asp Tyr Ala Phe Leu Met Glu Ser Thr
65                  70                  75                  80

Thr Ile Glu Phe Val Thr Gln Arg Asn Cys Asn Leu Thr Gln Ile Gly
                85                  90                  95

Gly Leu Ile Asp Ser Lys Gly Tyr Gly Val Gly Thr Pro Met Gly Ser
            100                 105                 110

Pro Tyr Arg Asp Lys Ile Thr Ile Ala Ile Leu Gln Leu Gln Glu Glu
        115                 120                 125

Gly Lys Leu His Met Met Lys Glu Lys Trp Trp Arg Gly Asn Gly Cys
    130                 135                 140

Pro Glu
145
```

(2) INFORMATION FOR SEQ ID NO:14:
- (i) SEQUENCE CHARACTERISTICS:
  - (A) LENGTH: 4 amino acids
  - (B) TYPE: amino acid
  - (C) STRANDEDNESS: single
  - (D) TOPOLOGY: linear
- (ii) MOLECULE TYPE: protein
- (iii) HYPOTHETICAL: NO
- (iv) ANTI-SENSE: NO
- (xi) SEQUENCE DESCRIPTION: SEQ ID NO:14

```
Pro Ala Val Ile
1
```

(2) INFORMATION FOR SEQ ID NO:15:
- (i) SEQUENCE CHARACTERISTICS:
  - (A) LENGTH: 7 amino acids
  - (B) TYPE: amino acid
  - (C) STRANDEDNESS: single
  - (D) TOPOLOGY: linear
- (ii) MOLECULE TYPE: protein
- (iii) HYPOTHETICAL: NO
- (iv) ANTI-SENSE: NO
- (xi) SEQUENCE DESCRIPTION: SEQ ID NO:15

```
Gly Ala Cys Ile Asp Leu Leu
1               5
```

(2) INFORMATION FOR SEQ ID NO:16:
- (i) SEQUENCE CHARACTERISTICS:
  - (A) LENGTH: 4 amino acids
  - (B) TYPE: amino acid
  - (C) STRANDEDNESS: single
  - (D) TOPOLOGY: linear
- (ii) MOLECULE TYPE: protein
- (iii) HYPOTHETICAL: NO
- (iv) ANTI-SENSE: NO
- (xi) SEQUENCE DESCRIPTION: SEQ ID NO:16

```
Gly Lys Ala Gly
1
```

(2) INFORMATION FOR SEQ ID NO:17:
- (i) SEQUENCE CHARACTERISTICS:
  - (A) LENGTH: 9 amino acids
  - (B) TYPE: amino acid
  - (C) STRANDEDNESS: single
  - (D) TOPOLOGY: linear
- (ii) MOLECULE TYPE: protein

(iii) HYPOTHETICAL: NO
(iv) ANTI-SENSE: NO
(xi) SEQUENCE DESCRIPTION: SEQ ID NO:17

Trp Asn Gly Met Ile Gly Glu Leu Val
1 5

(2) INFORMATION FOR SEQ ID NO:18:
(i) SEQUENCE CHARACTERISTICS:
(A) LENGTH: 10 amino acids
(B) TYPE: amino acid
(C) STRANDEDNESS: single
(D) TOPOLOGY: linear
(ii) MOLECULE TYPE: protein
(iii) HYPOTHETICAL: NO
(iv) ANTI-SENSE: NO
(xi) SEQUENCE DESCRIPTION: SEQ ID NO:18

Ala Asp Met Val Ala Pro Leu Thr Ile Asn
1 5 10

(2) INFORMATION FOR SEQ ID NO:19:
(i) SEQUENCE CHARACTERISTICS:
(A) LENGTH: 6 amino acids
(B) TYPE: amino acid
(C) STRANDEDNESS: single
(D) TOPOLOGY: linear
(ii) MOLECULE TYPE: protein
(iii) HYPOTHETICAL: NO
(iv) ANTI-SENSE: NO
(xi) SEQUENCE DESCRIPTION: SEQ ID NO:19

Glu Val Ile Asp Phe Ser
1 5

(2) INFORMATION FOR SEQ ID NO:20:
(i) SEQUENCE CHARACTERISTICS:
(A) LENGTH: 6 amino acids
(B) TYPE: amino acid
(C) STRANDEDNESS: single
(D) TOPOLOGY: linear
(ii) MOLECULE TYPE: protein
(iii) HYPOTHETICAL: NO
(iv) ANTI-SENSE: NO
(xi) SEQUENCE DESCRIPTION: SEQ ID NO:20

Gly Ile Ser Ile Met Val
1 5

(2) INFORMATION FOR SEQ ID NO:21:
(i) SEQUENCE CHARACTERISTICS:
(A) LENGTH: 4 amino acids
(B) TYPE: amino acid
(C) STRANDEDNESS: single
(D) TOPOLOGY: linear
(ii) MOLECULE TYPE: protein
(iii) HYPOTHETICAL: NO
(iv) ANTI-SENSE: NO
(xi) SEQUENCE DESCRIPTION: SEQ ID NO:21

Met Ala Xaa Met
1

(2) INFORMATION FOR SEQ ID NO:22:
(i) SEQUENCE CHARACTERISTICS:
(A) LENGTH: 4 amino acids
(B) TYPE: amino acid

(C) STRANDEDNESS: single
(D) TOPOLOGY: linear
(ii) MOLECULE TYPE: protein
(iii) HYPOTHETICAL: NO
(iv) ANTI-SENSE: NO
(xi) SEQUENCE DESCRIPTION: SEQ ID NO:22

Ala Phe Ile Ala
1

(2) INFORMATION FOR SEQ ID NO:23:
(i) SEQUENCE CHARACTERISTICS:
(A) LENGTH: 6 amino acids
(B) TYPE: amino acid
(C) STRANDEDNESS: single
(D) TOPOLOGY: linear
(ii) MOLECULE TYPE: protein
(iii) HYPOTHETICAL: NO
(iv) ANTI-SENSE: NO
(xi) SEQUENCE DESCRIPTION: SEQ ID NO:23

Ser Ala Val Leu Glu Ala
1 5

(2) INFORMATION FOR SEQ ID NO:24:
(i) SEQUENCE CHARACTERISTICS:
(A) LENGTH: 7 amino acids
(B) TYPE: amino acid
(C) STRANDEDNESS: single
(D) TOPOLOGY: linear
(ii) MOLECULE TYPE: protein
(iii) HYPOTHETICAL: NO
(iv) ANTI-SENSE: NO
(xi) SEQUENCE DESCRIPTION: SEQ ID NO:24

Ser Thr Gly Ala Gly Ile Ala
1 5

(2) INFORMATION FOR SEQ ID NO:25:
(i) SEQUENCE CHARACTERISTICS:
(A) LENGTH: 6 amino acids
(B) TYPE: amino acid
(C) STRANDEDNESS: single
(D) TOPOLOGY: linear
(ii) MOLECULE TYPE: protein
(iii) HYPOTHETICAL: NO
(iv) ANTI-SENSE: NO
(xi) SEQUENCE DESCRIPTION: SEQ ID NO:25

Leu Ala Ile Leu Gln Leu
1 5

## CLAIMS

I claim:

1. A method for designing a model of a protein-ligand binding pocket of a binding protein comprising

(a) building a model of the protein-ligand binding pocket based upon topographical similarity of the binding pocket to a bacterial periplasmic binding protein,

(b) refining the model of the binding pocket by energy minimization of the binding pocket with a high affinity ligand in the binding pocket,

(c) calculating interaction energies of basis set molecules by calculating the energies of the model of the binding pocket and the basis set molecules individually and the total energies of the individual bound complexes formed from the binding protein and the basis set molecules,

(d) generating a predictive equation by performing regression analysis on the calculated energies and on molecular characteristics of the basis set molecules, and

(e) altering the model of the binding pocket and repeating steps (b), (c), and (d) until either (1) the regression analysis results in a correlation coefficient of at least a predetermined value, or (2) none of the basis set molecules has a predicted $p(IC_{50})$ differing from an experimentally determined $p(IC_{50})$ by more than a predetermined value,

wherein when either (1) the regression analysis results in a correlation coefficient of at least the predetermined value, or (2) none of the basis set molecules has a predicted $p(IC_{50})$ differing from an experimentally determined $p(IC_{50})$ by more than the predetermined value, the predictive equation generated in the last iteration of step (d) is the final predictive equation and the model refined in the last iteration of step (b) is the final model.

2. The method of claim 1 further comprising

(f) calculating the interaction energy for a potential ligand molecule by calculating the energies of the binding pocket and the

potential ligand molecule individually and the energy of the bound complex formed from the binding pocket and the potential ligand molecule, and

(g) calculating the affinity of the potential ligand molecule by applying the interaction energies and molecular characteristics of the potential ligand molecule to the final predictive equation.

3. The method of claim 1 wherein the model of the binding pocket is altered to reduce or eliminate unfavorable contacts between the binding pocket and those basis set molecules having the greatest difference between the experimentally determined $p(IC_{50})$ and the predicted $p(IC_{50})$.

4. The method of claim 1 wherein the model is altered and steps (b), (c), and (d) are repeated until either the regression analysis results in a correlation coefficient of at least 0.8.

5. The method of claim 1 wherein the model is altered and steps (b), (c), and (d) are repeated until none of the basis set molecules has a predicted $p(IC_{50})$ differing from the experimentally determined $p(IC_{50})$ by more than 1.

6. The method of claim 1 wherein the model of the protein-ligand binding pocket is built based upon topographical similarity of the binding pocket to lysine/arginine/ornithine binding protein.

7. The method of claim 1 wherein the binding protein is a ligand gated ion channel protein, and wherein the model of the protein-ligand binding pocket is built based upon topographical similarity of the binding pocket to lysine/arginine/ornithine binding protein.

8. The method of claim 1 wherein the binding protein is a AMPA receptor,

wherein the model of the protein-ligand binding pocket is built based upon topographical similarity of the binding pocket to lysine/arginine/ornithine binding protein, and

wherein the model of the binding pocket is refined by energy minimization of the binding pocket with AMPA in the binding pocket.

9. The method of claim 1 wherein the binding protein is a kainate receptor,

wherein the model of the protein-ligand binding pocket is built based upon topographical similarity of the binding pocket to lysine/arginine/ornithine binding protein, and

wherein the model of the binding pocket is refined by energy minimization of the binding pocket with kainic acid in the binding pocket.

10. The method of claim 1 wherein the binding protein is an NMDA receptor,

wherein the protein-ligand binding pocket is a glutamate site on the NMDA receptor,

wherein the model of the binding pocket is built based upon topographical similarity of the binding pocket to lysine/arginine/ornithine binding protein, and

wherein the model of the binding pocket is refined by energy minimization of the binding pocket with glutamate in the binding pocket.

11. The method of claim 1 wherein the binding protein is an NMDA receptor,

wherein the protein-ligand binding pocket is a glycine site on the NMDA receptor,

wherein the model of the binding pocket is built based upon topographical similarity of the binding pocket to lysine/arginine/ornithine binding protein, and

wherein the model of the binding pocket is refined by energy minimization of the binding pocket with glycine in the binding pocket.

12. A method for predicting the selectivity of a potential ligand molecule for a set of related binding proteins having protein-ligand binding pockets, the method comprising

(a) building a model of each of the protein-ligand binding pockets based upon topographical similarity of the binding pockets to a bacterial periplasmic binding protein,

(b) refining the model of each of the binding pockets by energy minimization of the binding pockets with a high affinity ligand in the binding pockets,

(c) calculating interaction energies of basis set molecules by separately calculating the energies of the model of the binding pocket of each of the binding proteins and the basis set molecules individually and the total energies of the individual bound complexes formed from each of the binding proteins and the basis set molecules,

(d) generating a predictive equation for each of the binding proteins by performing regression analysis on the calculated energies and on molecular characteristics of the basis set molecules,

(e) refining the models of the binding pockets by, separately for each of the binding pockets,

altering the model of the binding pocket and repeating steps (b), (c), and (d) until either (1) the regression analysis results in a correlation coefficient of at least a predetermined value, or (2) none of the basis set molecules has a predicted $p(IC_{50})$ differing from $p(IC_{50})$ by more than a predetermined value,

wherein when either (1) the regression analysis results in a correlation coefficient of at least the predetermined value, or (2) none of the basis set molecules has a predicted $p(IC_{50})$ differing from $p(IC_{50})$ by more than the predetermined value, the predictive equation generated in the last iteration of step (d) is the final predictive equation and the model refined in the last iteration of step (b) is the final model,

(f) calculating the interaction energy for a potential ligand molecule by calculating the energies of each of the binding pockets and the potential ligand molecule individually and the energy of the bound complex formed from each of the binding pockets and the potential ligand molecule, and

(g) calculating the affinity of the potential ligand molecule for each of the binding pockets by applying the interaction energies and molecular

characteristics of the potential ligand molecule to each of the final predictive equations,

wherein a potential ligand molecule is considered selective if the difference between the calculated affinity of the potential ligand molecule for at least one of the binding pockets and the calculated affinity of the potential ligand molecule for at least one of the other binding pockets is greater than a predetermined value.

13. The method of claim 12 wherein each of the models is altered and steps (b), (c), and (d) are repeated until the regression analysis results in a correlation coefficient of at least 0.8.

14. The method of claim 12 wherein each of the models is altered and steps (b), (c), and (d) are repeated until none of the basis set molecules has a predicted $p(IC_{50})$ differing from $p(IC_{50})$ by more than 1.

15. A method for predicting the affinity of a potential ligand molecule binding to a binding protein having a protein-ligand binding pocket, the method comprising

(a) calculating the interaction energy for a potential ligand molecule by calculating the energies of a model of the protein-ligand binding pocket and the potential ligand molecule individually and the energy of the bound complex formed from the binding pocket and the potential ligand molecule, and

(b) calculating the affinity of the potential ligand molecule by applying the interaction energies and molecular characteristics of the potential ligand molecule to a predictive equation for ligand binding to the binding protein,

wherein (1) the binding protein is AMPA receptor GluR3 and the model of the binding protein is the model of Table 3, (2) the binding protein is NMDA receptor NR2-B and the model of the binding protein is the model of Table 4, (3) the binding protein is kainate receptor GluR6 and the model of the binding protein is the model of Table 5, or (4) the binding protein is NMDA receptor NR1 and the model of the binding protein is the model of Table 6.

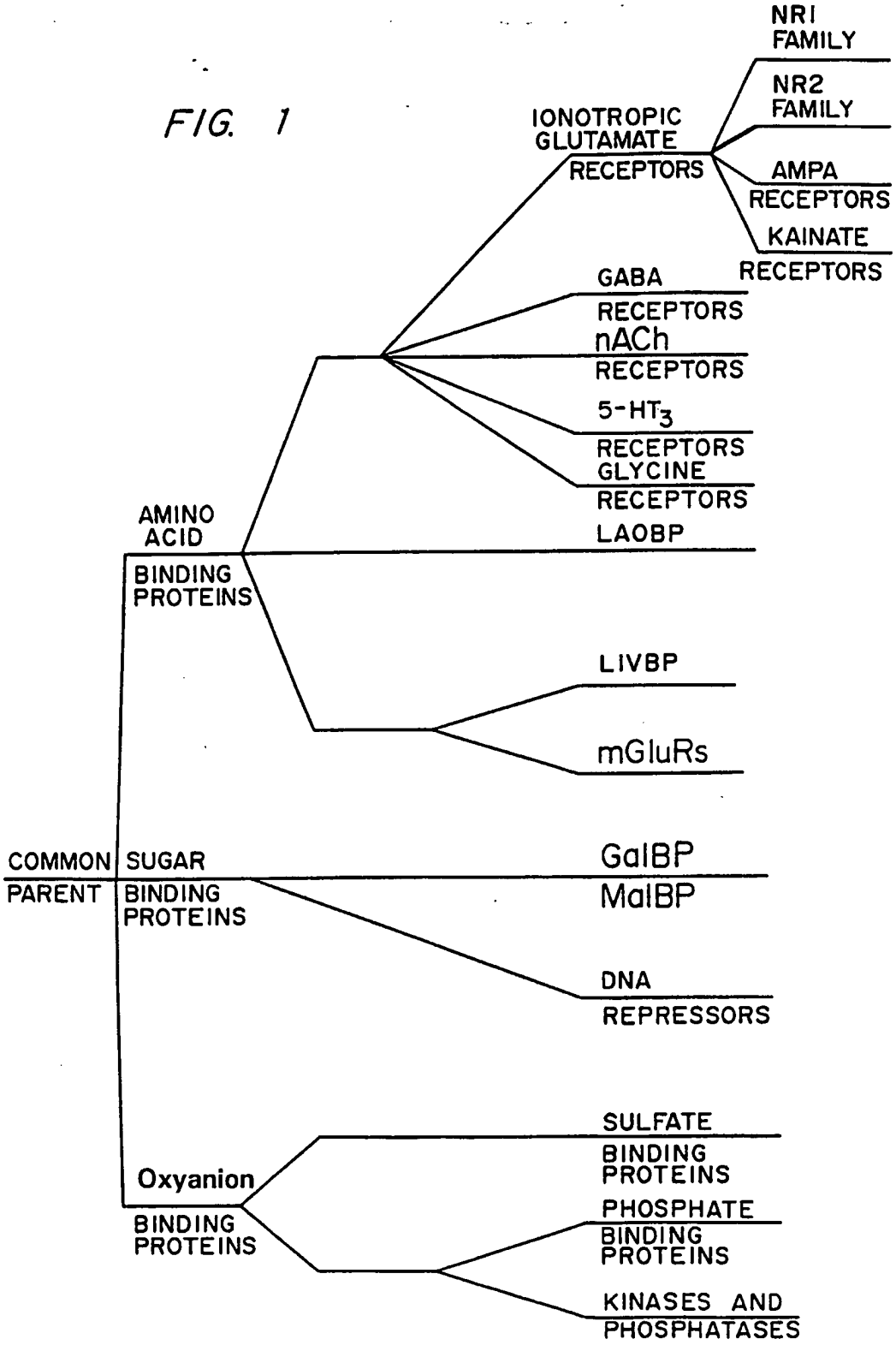
16. The method of claim 15 wherein the the binding protein is AMPA receptor GluR3 and the model of the binding protein is the model of Table 3.

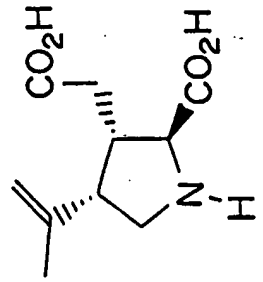
17. The method of claim 15 wherein the binding protein is NMDA receptor NR2-B and the model of the binding protein is the model of Table 4.

18. The method of claim 15 wherein the binding protein is kainate receptor GluR6 and the model of the binding protein is the model of Table 5.

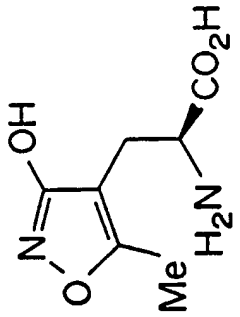
19. The method of claim 15 wherein the binding protein is NMDA receptor NR1 and the model of the binding protein is the model of Table 6.

FIG. 1

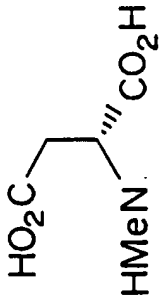

COMMON PARENT
AMINO ACID BINDING PROTEINS
IONOTROPIC GLUTAMATE RECEPTORS
NR1 FAMILY
NR2 FAMILY
AMPA RECEPTORS
KAINATE RECEPTORS
GABA RECEPTORS
nACh RECEPTORS
5-HT3 RECEPTORS
GLYCINE RECEPTORS
LAOBP
LIVBP
mGluRs
SUGAR BINDING PROTEINS
GalBP
MalBP
DNA REPRESSORS
Oxyanion BINDING PROTEINS
SULFATE BINDING PROTEINS
PHOSPHATE BINDING PROTEINS
KINASES AND PHOSPHATASES



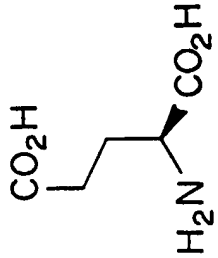

Kainic Acid




S-AMPA




NMDA




L-glutamate

FIG. 2

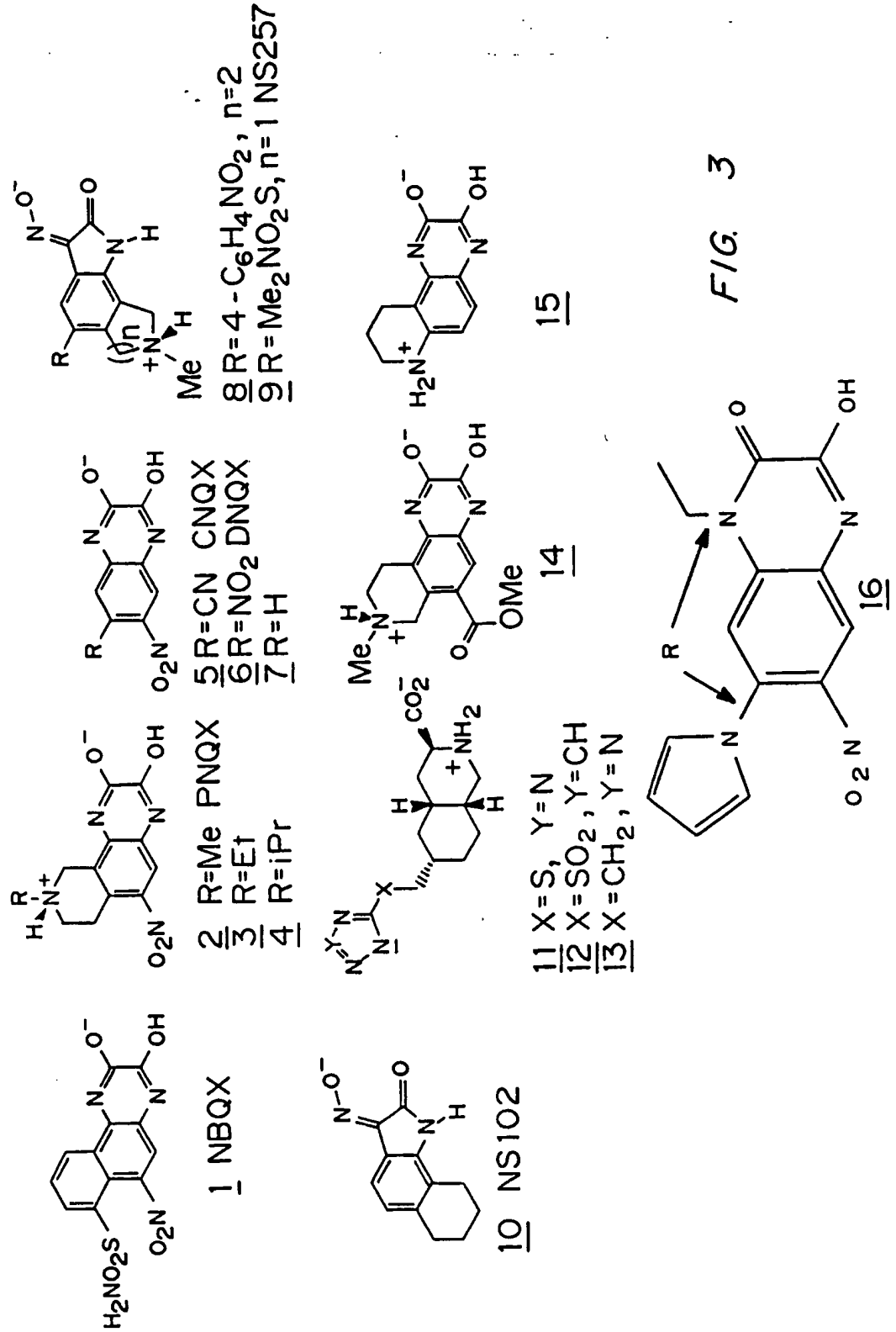
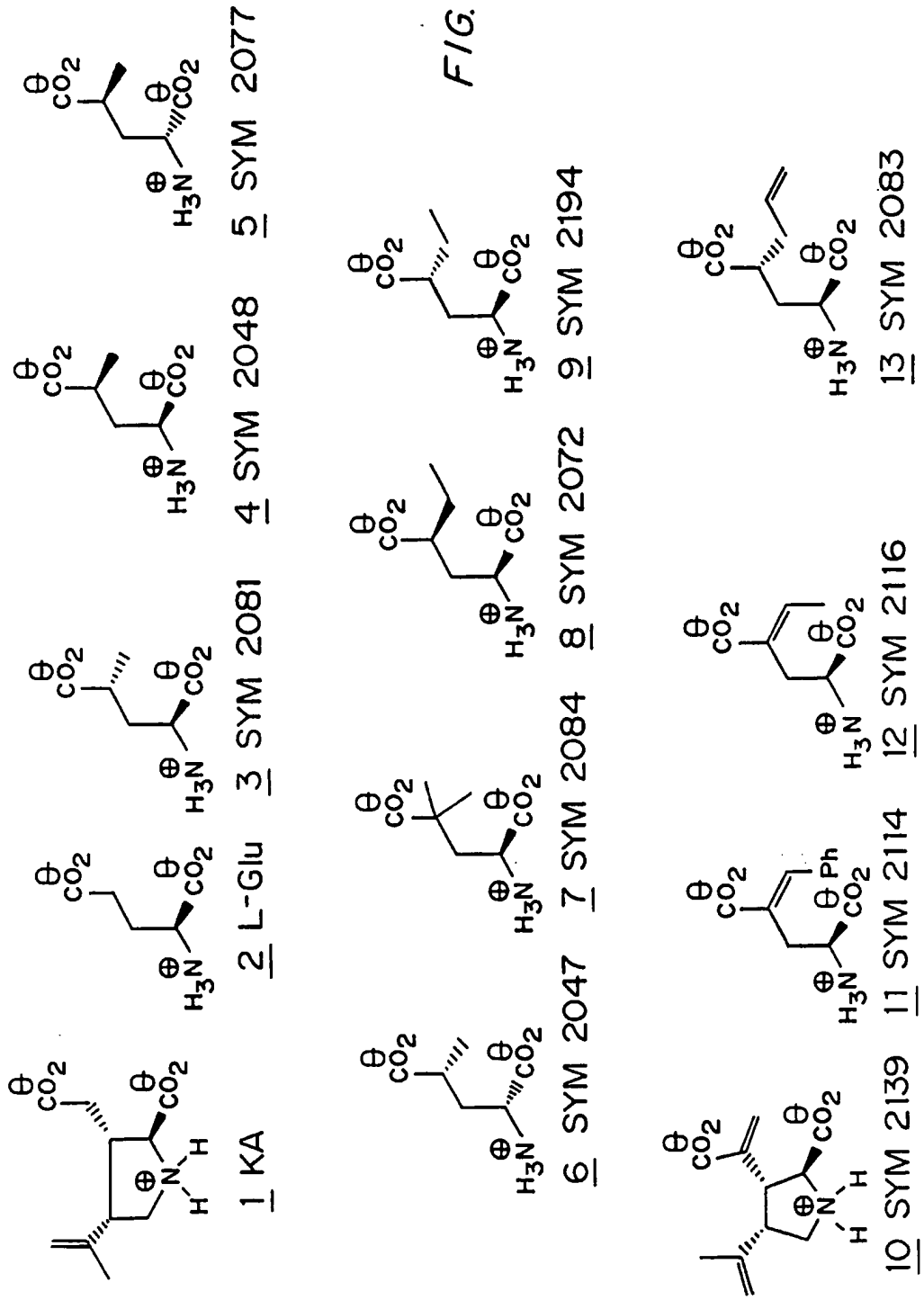
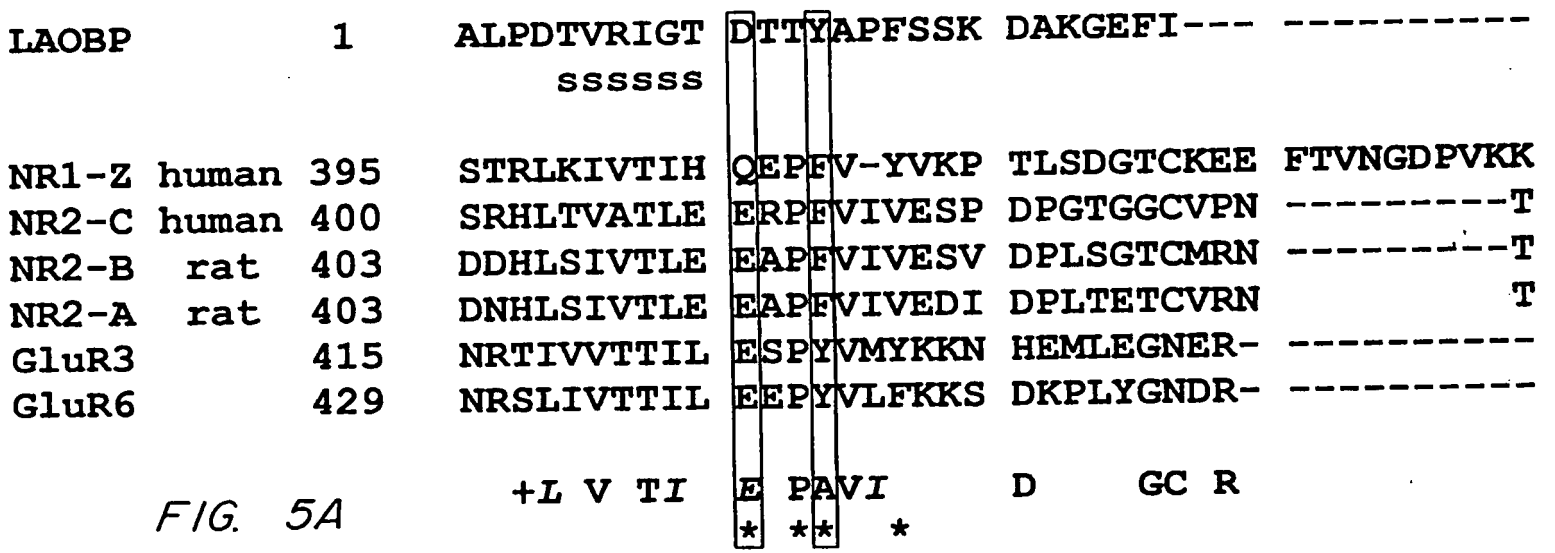

1 NBQX
2 R=Me PNQX
3 R=Et
4 R=iPr
5 R=CN CNQX
6 R=NO2 DNQX
7 R=H
8 R=4-C6H4NO2, n=2
9 R=Me2NO2S, n=1 NS257
10 NS102
11 X=S, Y=N
12 X=SO2, Y=CH
13 X=CH2, Y=N
14
15
16

FIG. 3

FIG. 4


1 KA
2 L-Glu
3 SYM 2081
4 SYM 2048
5 SYM 2077
6 SYM 2047
7 SYM 2084
8 SYM 2072
9 SYM 2194
10 SYM 2139
11 SYM 2114
12 SYM 2116
13 SYM 2083



```
LAOBP          1    ALPDTVRIGT DTTYAPFSSK DAKGEFI--- ----------
                        ssssss

NR1-Z human  395    STRLKIVTIH QEPFV-YVKP TLSDGTCKEE FTVNGDPVKK
NR2-C human  400    SRHLTVATLE ERPFVIVESP DPGTGGCVPN ----------T
NR2-B  rat   403    DDHLSIVTLE EAPFVIVESV DPLSGTCMRN ----------T
NR2-A  rat   403    DNHLSIVTLE EAPFVIVEDI DPLTETCVRN           T
GluR3        415    NRTIVVTTIL ESPYVMYKKN HEMLEGNER- ----------
GluR6        429    NRSLIVTTIL EEPYVLFKKS DKPLYGNDR- ----------

                    +L V TI  E PAVI      D     GC R
                             *  **  *
```

FIG. 5A

```
LAOBP          28   ---------- ---------- -----GFDID LGNEMCKRMQ
                                           hhhhh hhhhhhhhh

NR1-Z human  434    VICTGPNDTS PGSPRH-TVP -QCCYGFCID LLIKLARTMN
NR2-C human  431    VPCRRQSNHT FSSGDVAPYT KLCCKGFCID ILKKLARVVK
NR2-B  rat   434    VPCQKRIISE NKTDEEPGYI KKCCKGFCID ILKKISKSVK
NR2-A  rat   434    VPCRKFVKIN NSTNEGMNV- KKCCKGFCID ILKKLSRTVK
GluR3        444    ---------- ---------- ---YEGYCVD LAYEIAKHVR
GluR6        458    ---------- ---------- ---FEGYCID LLRELSTILG

                    V C +                 K CC GACID LL KLA+ V+
```

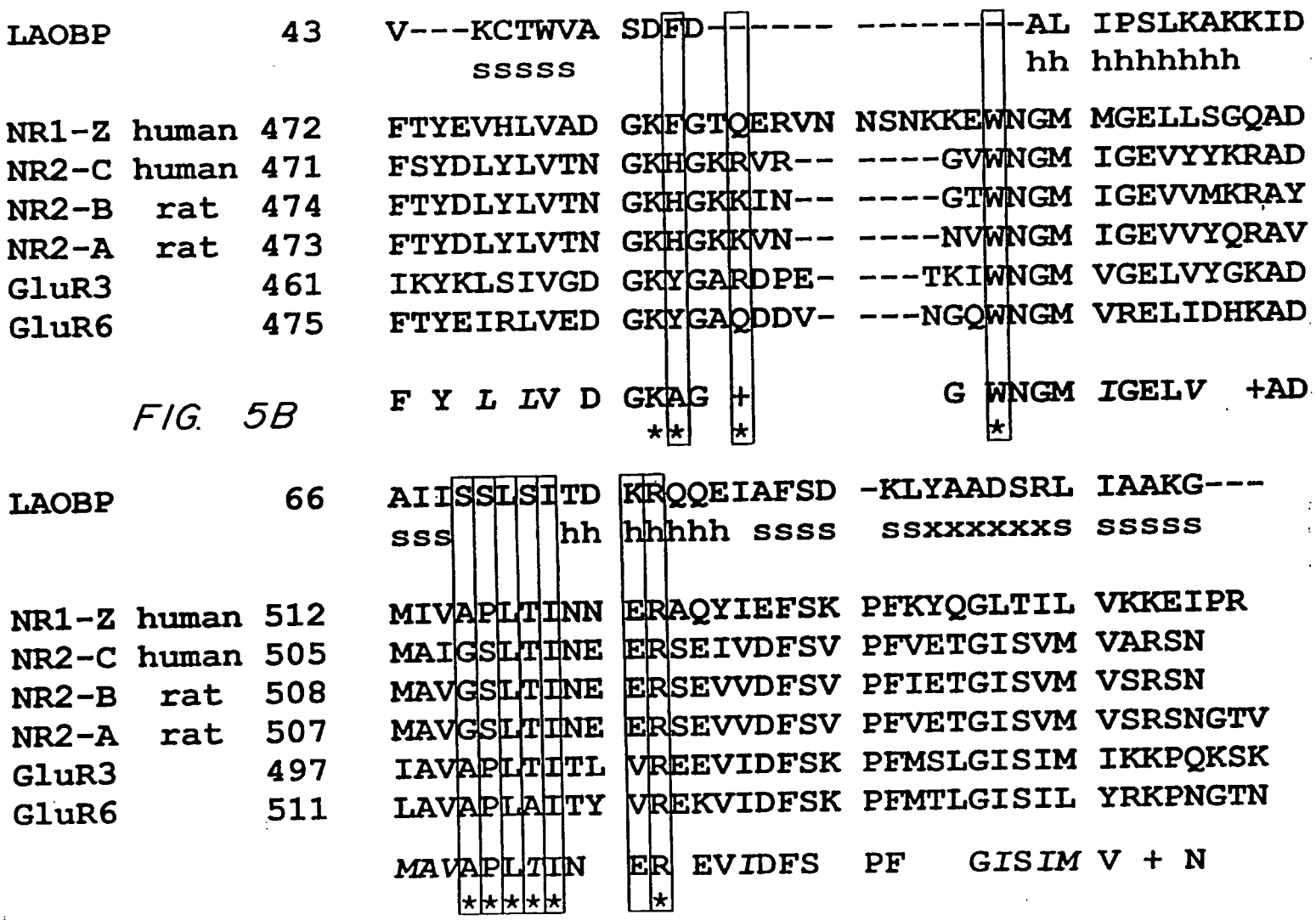



FIG. 5B

```
LAOBP          100   ----SPVQ-P TLESLKG--- KHVGVLQGST QEAYANDNWR
                           hhhh        ssssss    hhhhhhhh

NR1-Z human    665   TGINDPRLRN P--SDK---F IYATVKQSSV DIYFRRQVE-
NR2-C human    666   KKFQRPQDQY PP-------F RFGTVPNGST ERNIRSNY--
NR2-B  rat     669   KKFQRPNDFS PP-------F RFGTVPNGST ERNIRNNY--
NR2-A  rat     668   KKFQRPHDYS PP-------F RFGTVPNGST ERNIRNNY--
GluR3          652   ERMVSPIE-S AEDLAKQETI AYGTLDSGST KEFFRRSKIA
GluR6          660   ERMESPID-S ADDLAKQTKI EYGAVEDGAT MTFFKKSKIS

FIG. 5C              +   P D S P    K   F  AGTV  GST   AF+
                                                 ***

LAOBP          132   -TKGVDVVAY ANQD----LI YSDLTAGRLD AALQ-DEVAA
                         ssssss      hh hhhhhh     ssss   hhh

NR1-Z human    699   -LSTMYRHME KHNY----ES AAEAIQAVRD NKLH-AFIWD
NR2-C human    697   --RDMHTHMV KFNQ----RS VEDALTSLKM GKLD-AFIYD
NR2-B  rat     700   --AEMHAYMG KFNQ----RG VDDALLSLKT GKLD-AFIYD
NR2-A  rat     699   --PYMHQYMT RFNQ----RG VEDALVSLKT GKLD-AFIYD
GluR3          691   VYEKMWSYMK SAEPSVFTKT TADGVARVRK SKGKFAFLLE
GluR6          699   TYDKMWAFMS SRRQSVLVKS NEEGIQRV-- LTSDYAFLME

                     MArAM  +ANQ    +S  --AL  V+   KLD AFIA-
```

```
LAOBP          166   SEGFLKQPAG KEYAFAGPSV -KDKKYFGDG TGVGLRKDDT
                     hhhhhh       ssss       xxxxxx        ssss

NR1-Z human    733   SAVLEFE--- ASQKCDLVT- -TGELFFRSG FGIGMRK-DS
NR2-C human    730   AAVLNYM-AG KDEGCKLVTI GSGKVFATTG YGIAMQK-DS
NR2-B  rat     733   AAVLNYM-AG RDEGCKLVT- -SGKVFASTG YGIAIQK-DS
NR2-A  rat     732   AAVLNYK-AG RDEGCKLVTI GSGYIFASTG YGIALQK-GS
GluR3          731   STMNEYI--E QRKPCDTMK- -VGGNLDSKG YGVATPK-GS
GluR6          737   STTIEFV--T QRN-CNLTQ- -IGGLIDSKG YGVGTPM-GS

    FIG. 5D          SAVLEAr        C LVT    G   F STG AGIA  K DS
                                    *            *   *

LAOBP          205   ELKAAFDKAL TELRQDGTYD KMAKKYF-DF NVYGD
                      hhhhhhhhh hhhhh  hhh hhhhhh

NR1-Z human    767   PWKQNVSLSI LKSHENGFME DLDKTWV-RY QECDS
NR2-C human    769   HWKRAIDLAL LQFLGDGETQ KLETVWL--S GICQN
NR2-B  rat     769   GWKRQVDLAI LQLFGDGEME ELEALWL--T GICHN
NR2-A  rat     770   PWKRQIDLAL LQFVGDGEME ELETLWL--T GICHN
GluR3          766   ALGNAVNLAV LKLNEQGLLD KLKNKWWYDK GECGS
GluR3          771   PYRDKITIAI LQLQEEGKLH MMKEKWW-RG NGCPE

                     ArK  V LAI LQL E G M   L   W     G C
```

```
LAOBP    1    ALPDTVRIGT DTTYAP--FS SKD-----AK GEFIGFDIDL
                  ssssss                          hhhhhhh

GluR3  412    SSENRTIVVT TILESPYVMY KKNHEMLEGN ERYEGYCVDL
GluR6  426    SLSNRSLIVT TILEEPYVLF KKSDKPLYGN DRFEGYCIDL

LAOBP   34    GNEMCKRMQV KCTWV-ASDF DALIPSLKAK KI--------
              hhhhhhhh   sssss        hhhhhhhhh          h
GluR3  452    AYEIAKHVRI KYKLSIVGDG KYGARDPETK IWNGMVGELV
GluR6  466    LRELSTILGF TYEIRLVEDG KYGAQDDVNG QWNGMVRELI

LAOBP   65    ----DAIISS LSITDKRQQE IAFSD-KLYA ADSRLIAAKG
                   sss      hhhhhhh  ssss ssxx xxxxsssssss
GluR3  492    YGKADIAVAP LTITLVREEV IDFSKPFMSL GISIMIKKPQ
GluR6  506    DHKADLAVAP LAITYVREKV IDFSKPFMTL GISILYRKPN

LAOBP  100    ---SPVQ-PT LESLKG---K HVGVLQGSTQ EAYANDNWR-
                         hhhh     s sssss    h hhhhhhh
GluR3  651    VERMVSPIES AEDLAKQETI AYGTLDSGST KEFFRRSKIA
GluR6  659    VERMESPIDS ADDLAKQTKI EYGAVEDGAT MTFFKKSKIS
```

FIG. 6A

```
LAOBP 132    -TKGVDVVAY A---------N QDLIYSDLTA GRLDAALQDE
                 ssssss               hhhhhhhh     ssss
GluR3 691    VYEKMWSYMK SAEPSVFTKT TADGVARVRK SKGKFAFLL-E
GluR6 699    TYDKMWAFMS SRRQSVLVKS NEEGIQRVLT S--DYAFLM-E

LAOBP 163    VAASEGFLKQ PAGKEYAFAG PSVKDKKYFG DGTGVGLRKD
             hhhhhhhhh      ssss     xxxxx      ssss
GluR3 731    STMNEYIEQR KPC--DTMKV GGNL----DS KGYGVATPK-
GluR6 737    STTIEFVTQR N-C--NLTQI GGLI----DS KGYGVGTPM-

LAOBP 203    DTELKAAFDK ALTELRQDGT YDKMAKKYFD FNVYGD
                hhhhhhh hhhhhhh  h hhhhhhhh
GluR3 764    GSALGNAVNL AVLKLNEQGL LDKLKNKWWY DKGECG
GluR6 769    GSPYRDKITI AILQLQEEGK LHMMKEKWW- RGNGCP
```

FIG. 6B